

mino acid sequence for full length human wild type EPHA2 [SEQ. ID No. 1] [SEQ

<u>ID NO: 1</u>]

(Residues 596-900 are underlined)

MELQAARACFALLWGCALAAAAAAQGKEVVLLDFAAAGGELGWLTHPYGK	50
GWDLMQNIMNDMPIYMYSVCNVMSGDQDNWLRTNWVYRGEAERNNFELNF	100
TVRDCNSFPGGASSCKETFNLYYAESDLDYGTNFQKRLFTKIDTIAPDEI	150
TVSSDFEARHVKLNVEERSVGPLTRKGFYLAFQDIGACVALLSVRVYYKK	200
CPELLQGLAHFPETIAGSDAPSLATVAGTCVDHAVVPPGGEEPRMHCAVD	250
GEWLVPIGQCLCQAGYEKVEDACQACSPGFFKFEASESPCLECPEHTLPS	300
PEGATSCECEEGFFRAPQDPASMPCTRPPSAPHYLTAVGMGAKVELRWTP	350
PQDSGGREDIVYSVTCEQCWPESGECGPCEASVRYSEPPHGLTRTSVTVS	400
DLEPHMNYTFTVEARNGVSGLVTSRSFRTASVSINQTEPPKVRLEGRSTT	450
SLSVSWSIPPPQQSRVWKYEVTYRKKGDSNSYNVRRTEGFSVTLDDLAPD	500
TTYLVQVQALTQEGQGAGSKVHEFQTLSPEGSGNLAVIGGVAVGVVLLLV	550
LAGVGFFIHRRRKNQRARQSPEDVYFSKSEQLKPLKTYVDPHTYE <u>DPNQA</u>	600
VLKFTTEIHPSCVTRQKVIGAGEFGEVYKGMLKTSSGKKEVPVAIKTLKA	650
GYTEKQRVDFLGEAGIMGQFSHHNIIRLEGVISKYKPMMIITEYMENGAL	700
<u>DKFLREKDGEFSVLQLVGMLRGIAAGMKYLANMNYVHRDLAARNILVNSN</u>	750
LVCKVSDFGLSRVLEDDPEATYTTSGGKIPIRWTAPEAISYRKFTSASDV	800
WSFGIVMWEVMTYGERPYWELSNHEVMKAINDGFRLPTPMDCPSAIYQLM	850
MQCWQQERARRPKFADIVSILDKLIRAPDSLKTLADFDPRVSIRLPSTSG	900
SEGVPFRTVSEWLESIKMQQYTEHFMAAGYTAIEKVVQMTNDDIKRIGVR	950
LPGHQKRIAYSLLGLKDQVNTVGIPI	976

FIGURE 1A (Cont.)

Human cDNA sequence encoding residues 596-900 of EPHA2 [SEQ. ID No. 2] [SEQ ID NO: 2]

GACCCCAACCAGGCTGTTTGAAGTTCACTACCGAGATCCATCC	50
TGTCACTCGGCAGAAGGTGATCGGAGCAGGAGAGTTTGGGGAGGTGTACA	100
AGGGCATGCTGAAGACATCCTCGGGGAAGAAGGAGGTGCCGGTGGCCATC	150
AAGACGCTGAAAGCCGGCTACACAGAGAAGCAGCGAGTGGACTTCCTCGG	200
CGAGGCCGGCATCATGGGCCAGTTCAGCCACCACAACATCATCCGCCTAG	250
AGGGCGTCATCTCCAAATACAAGCCCATGATGATCATCACTGAGTACATG	300
GAGAATGGGGCCCTGGACAAGTTCCTTCGGGAGAAGGATGGCGAGTTCAG	350
CGTGCTGCAGCTGGGGCATGCTGCGGGGCATCGCAGCTGGCATGAAGT	400
ACCTGGCCAACATGAACTATGTGCACCGTGACCTGGCTGCCCGCAACATC	450
CTCGTCAACAGCAACCTGGTCTGCAAGGTGTCTGACTTTGGCCTGTCCCG	500
CGTGCTGGAGGACCCCGAGGCCACCTACACCACCAGTGGCGGCAAGA	550
TCCCCATCCGCTGGACCGCCCCGGAGGCCATTTCCTACCGGAAGTTCACC	600
TCTGCCAGCGACGTGTGGAGCTTTGGCATTGTCATGTGGGAGGTGATGAC	650
CTATGGCGAGCGCCCTACTGGGAGTTGTCCAACCACGAGGTGATGAAAG	700
CCATCAATGATGGCTTCCGGCTCCCCACACCCATGGACTGCCCCTCCGCC	750
ATCTACCAGCTCATGATGCAGTGCTGGCAGCAGGAGCGTGCCCGCCC	800
CAAGTTCGCTGACATCGTCAGCATCCTGGACAAGCTCATTCGTGCCCCTG	850
ACTCCCTCAAGACCCTGGCTGACTTTGACCCCCGCGTGTCTATCCGGCTC	900
CCCAGCACGAGCGGC	• 915

Amino acid sequence for residues 596-900 of EPHA2 with a cleavable (rTev) N-terminal 6x-histidine tag [SEQ. ID No. 3] [SEQ ID NO: 3] (6x-histidine tag and cleavage site are underlined)

MSYYHHHHHHDYDIPTTENLYFQGAMGSDPNQAVLKFTTEIHPSCVTRQK	50
VIGAGEFGEVYKGMLKTSSGKKEVPVAIKTLKAGYTEKQRVDFLGEAGIM	100
GQFSHHNIIRLEGVISKYKPMMIITEYMENGALDKFLREKDGEFSVLQLV	150
GMLRGIAAGMKYLANMNYVHRDLAARNILVNSNLVCKVSDFGLSRVLEDD	200
PEATYTTSGGKIPIRWTAPEAISYRKFTSASDVWSFGIVMWEVMTYGERP	250
YWELSNHEVMKAINDGFRLPTPMDCPSAIYQLMMQCWQQERARRPKFADI	. 300
VSILDKLIRAPDSLKTLADFDPRVSIRLPSTSG	333

FIGURE 3A

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number' (SEQ ID NO: 1), (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	В	С	D	E	F	G	Н	I	J
1	N	ALA	Α	605	47.239	45.529	67.448	1.00	51.83
2	CA	ALA			46.929	45.860	66.049	1.00	
3	CB			605	45.751	44.876	65.490		51.40
4	C			605	46.433	47.259	66.307		51.78
5	Ō			605	46.252	47.630	67.422	1.00	
6	N			606	46.218	48.048	65.302	1.00	
7	CA			606	45.719	49.337	65.564		49.98
8	СВ			606	46.128	50.120	64.454	1.00	
9	OG1			606	47.553	50.041	64.401	1.00	
10	CG2	THR	Α	606	45.766	51.541	64.651	1.00	48.25
11	С	THR	Α	606	44.201	49.397	65.650	1.00	50.57
12	0	THR	Α	606	43.487	48.868	64.787	1.00	51.60
13	N	GLU	Α	607	43.680	50.086	66.646	1.00	49.68
14	CA	GLU	Α	607	42.264	50.182	66.717	1.00	47.97
15	CB	GLU	Α	607	41.796	50.123	68.130	1.00	47.41
16	CG	GLU	Α	607	40.323	50.414	68.279	1.00	50.07
17	CD	GLU	Α	607	39.394	49.230	68.074	1.00	39.82
18	OE1	GLU	Α	607	39.796	48.072	68.195	1.00	38.52
19	OE2	GLU	Α	607	38.260	49.515	67.856	1.00	41.61
20	C.	GLU			41.841	51.347	65.971		48.16
21	0			607	42.392	52.398	66.162		48.74
22	N			608	40.955	51.146	64.963	1.00	
23	CA			608	40.531	52.309	64.228		49.42
24	CB			608	41.128	52.517	62.742		51.19
25	CG1			608	40.066	52.886	61.752	1.00	
26	CD1			608	39.259	51.726	61.615		60.72
27	CG2			608	42.168	51.494	62.300		47.67
28	C	ILE			39.135	52.787	64.481	1.00	
29	0	ILE			38.254	52.049	64.879	1.00	
30	N	HIS			38.983	54.090	64.361	1.00	
31	CA	HIS			37.727	54.745	64.674	1.00	
32	CB	HIS			37.938	56.203	65.196		57.26
33	CG	HIS			36.715	56.776	65.835	1.00	
34 35		HIS HIS			36.486	56.686	67.186	1.00	62.57 62.48
36	NE2	HIS			35.313	57.221 57.635	67.471	1.00	
37	CD2	HIS			34.764 35.606	57.635 57.345	66.348 65.301	1.00	
38	CDZ	HIS			36.701	54.718	63.557		53.34
39	0	HIS			36.701	55.109	62.474		55.03
40	N	PRO			35.517	54.263	63.854	1.00	
41	CA	PRO			34.533	54.203	62.805	1.00	53.20
42	CB	PRO			33.246	53.864	63.591	1.00	52.67
43	CG	PRO			33.753	53.087	64.713	1.00	50.94

FIGURE 3A (Cont.)

A	В	С	D	E	F	G	Н	I.	J
4.4	an.	DDO	70	610	35 060	E3 693	6E 122	1 00	E2 00
44	CD			610	35.069	53.682	65.133		52.08
45	C			610	34.421	55.273	61.903	1.00	
46	0			610	33.935	55.146	60.793	1.00	
47	N			611	34.789	56.418	62.391		52.17
48	CA			611	34.546	57.584	61.639		52.33
49	CB	SER			34.694	58.833	62.562		54.93
50	OG			611	35.822	58.723	63.443		49.81
51	C	SER			35.579	57.611	60.552	1.00	
52	0	SER			35.394	58.256	59.545	1.00	
53	N	CYS			36.679	56.915	60.701	1.00	
54	CA			612	37.633	57.083	59.642		51.06
55	CB	CYS	Α	612	39.044	56.889	60.169	1.00	50.65
56	SG	CYS	Α	612	39.193	57.805	61.702	1.00	55.75
57	С	CYS	Α	612	37.445	56.214	58.426	1.00	49.07
58	0	CYS	Α	612	38.215	56.286	57.479	1.00	48.12
59	N	VAL	Α	613	36.470	55.349	58.497	1.00	49.20
60	CA	VAL	Α	613	36.329	54.361	57.471	1.00	48.42
61	CB	VAL	Α	613	36.130	52.976	58.087	1.00	49.58
62	CG1	VAL	Α	613	35.493	52.026	57.030	1.00	46.32
63	CG2	VAL	Α	613	37.477	52.423	58.651	1.00	46.61
64	С	VAL	Α	613	35.039	54.652	56.779	1.00	47.49
65	0	VAL	Α	613	34.080	55.078	57.401	1.00	46.54
66	N	THR			34.976	54.426	55.496	1.00	46.87
67	CA	THR			33.674	54.449	54.961		47.76
68	CB	THR			33.230	55.839	54.547		48.10
69	OG1	THR			32.501	55.759	53.312	1.00	
70	CG2	THR			34.430	56.804	54.383	1.00	
71	C	THR			33.479	53.362	53.956		47.36
72	ō	THR			34.145	53.317	52.971		49.44
73	N	ARG			32.519	52.496	54.192		46.37
74	CA	ARG			32.356	51.360	53.352		44.80
75	CB	ARG			31.323	50.464	53.993		43.89
76	CG	ARG			31.817	49.366	54.921		44.82
77	CD	ARG			30.699	48.434	55.297		45.58
78	NE	ARG			29.827	49.226	56.142		49.04
79	CZ	ARG			29.151	48.769	57.151	1.00	
80	NH1	ARG			29.164	47.437	57.427		50.76
						49.652			
81 82	NH2 C	ARG ARG			28.473		57.883		51.85
83	0	ARG			31.694	51.886 52.603	52.150		45.54
		GLN			30.737		52.357		47.25
84	N				32.035	51.399	50.944		45.88
85	CA	GLN			31.366	51.824	49.681		46.97
86	CB	GLN			32.323	52.657	48.734		47.24
87	CG	GLN			33.258	53.608	49.475		49.82
88	CD	GLN			34.200	54.437	48.588		55.54
89	OE1	GLN			35.203	53.909	48.073		56.72
90	NE2	GLN			33.889	55.770	48.428		56.51
91	C .	GLN			30.597	50.752	48.848		46.63
92	0	GLN			29.448	50.970	48.361		48.68
93	N	LYS			31.167	49.598	48.678		44.77
94	CA	LYS			30.497	48.628	47.857		44.21
95	CB	LYS	А	617	30.835	48.787	46.331	1.00	44.70

FIGURE 3BA (Cont.)

A	В	С	D	E	F	G	H	I	J
96	CG	LYS	Α	617	32.399	48.959	45.944	1.00	48.09
97	CD	LYS			32.768	48.759	44.391	1.00	58.41
98	CE			617	34.285	49.300	44.085	1.00	60.72
99	NZ			617	35.073	48.944	42.813	1.00	59.09
100	C			617	31.019	47.331	48.370		43.38
101	Ō			617	32.139	47.297	48.834		42.92
102	N			618	30.126	46.333	48.379		42.86
103	CA			618	30.376	44.945	48.657		41.23
104	СВ			618	29.070	44.146	48.522		39.95
105		VAL			29.426	42.622	48.582		40.13
106	CG2	VAL			28.147	44.503	49.610		42.60
107	C			618	31.203	44.381	47.543		40.46
108	ō			618	30.854	44.667	46.392		42.70
109	N			619	32.237	43.567	47.809		37.69
110	CA			619	33.059	43.022	46.731		33.98
111	CB			619	34.521	43.786	46.495		36.65
112	CG1			619	35.584	43.320	47.540		31.94
113	CD1			619	36.383	44.380	48.493		29.73
114	CG2			619	34.380	45.336	46.302		31.41
115	C			619	33.357	41.588	46.995		33.91
116	ō			619	34.185	41.024	46.280		35.83
117	N			620	32.752	40.970	47.989		32.82
118	CA			620	33.039	39.577	48.271		32.89
119	C			620	32.373	39.194	49.553		32.89
120	0			620	31.714	39.949	50.177		30.70
121	N			621	32.511	37.954	49.897		34.15
122	CA			621	31.818	37.384	51.019		35.78
123	CB			621	30.777	36.453	50.533		35.84
124	C			621	32.833	36.551	51.687		37.56
125	Ō			621	33.491	35.782	51.007		39.38
126	N			622	33.026	36.691	52.986		38.91
127	CA			622	34.006	35.848	53.611		38.65
128	C			622	33.398	34.928	54.575		39.55
129	0			622	32.173	34.902	54.796		36.11
130	N	GLU	Α	623	34.293	34.225	55.272		41.01
131	CA			623	33.843	33.363	56.342		41.61
132	CB	GLU	Α	623	35.046	32.793	57.068		43.27
133	CG	GLU	Α	623	34.682	31.885	58.223	1.00	50.78
134	CD			623		31.063	58.780	1.00	65.56
135	OE1	GLU	Α	623	36.962	31.030	58.200	1.00	64.79
136	OE2	GLU	Α	623	35.592	30.422	59.836		72.34
137	С	GLU	Α	623	32.965		57.417		40.39
138	0	GLU	Α	623		33.457	57.987	1.00	38.12
139	N	PHE	Α	624	33.265	35.347	57.758	1.00	37.75
140	CA	PHE	Α	624	32.522	35.965	58.889	1.00	36.41
141	CB	PHE	Α	624	33.506	36.538	59.933	1.00	37.60
142	CG	PHE	Α	624	34.593	35.546	60.354	1.00	34.22
143	CD1	PHE	Α	624	34.285	34.584	61.169	1.00	32.75
144	CE1	PHE	Α	624	35.256	33.643	61.527		42.16
145	CZ	PHE	A	624	36.568	33.666	61.022	1.00	37.78
146	CE2	PHE	Α	624	36.866	34.594	60.168	1.00	37.66
147	CD2	PHE	Α	624	35.861	35.571			37.30

FIGURE 3AP LECEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

Α	В	С	D	E	F	G	Н	I	J
2057	N	ΔΤ.Δ	R	602	61.588	-1.705	97.096	1.00	75.62
2058	CA			602	61.031	-2.970	96.546	1.00	76.68
2059	CB			602	61.665	-3.292	95.199	1.00	76.47
2060	C	ALA			61.337	-4.080	97.519		77.44
2061	ō	ALA			61.332	-5.311	97.156		75.75
2062	N			603	61.635	-3.605	98.744	1.00	77.75
2063	CA	LYS			62.173	-4.417	99.861	1.00	77.56
2064	CB			603	63.425	-3.748	100.411	1.00	78.96
2065	CG	LYS			63.212	-2.282	100.938	1.00	78.12
2066	CD			603	62.779		102.422	1.00	78.99
2067	CE	LYS			63.952		103.426	1.00	79.93
2068	NZ			603	64.536		103.573	1.00	79.82
2069	C			603	61.103		100.921	1.00	76.81
2070	0			603	61.315		102.072	1.00	75.16
2071	N			604	59.938		100.457	1.00	76.03
2072	CA			604	58.711		101.207	1.00	
2073	CB			604	58.102		100.991	1.00	
2074	CG			604	58.700		101.857	1.00	78.39
2075	CD1				58.564		103.231	1.00	
2076	CE1			604	59.115		104.059		84.10
2077	CZ			604	59.854		103.511		81.74
2078	CE2	PHE			60.017		102.144		82.47
2079	CD2	PHE			59.448	-0.503	101.312		81.05
2080	C			604	57.783		100.707		73.54
2081	Ō			604	56.553		100.826		73.46
2082	N			605	58.368	-6.069	100.190		71.71
2083	CA			605	57.496	-7.068	99.640		68.96
2084	СВ	THR			57.540	-6.922	98.163		68.75
2085	OG1	THR			57.203	-8.191	97.632		71.34
2086	CG2	THR			58.991	-6.774	97.722		71.15
2087	C	THR			57.874	-8.494	99.969		65.74
2088	0	THR			59.000	-8.868	99.864		66.65
2089	N	THR			56.897		100.339		61.47
2090	CA			606	57.083				56.89
2091	СВ	THR			55.818		101.234	1.00	
2092	OG1	THR			55.636		102.470		53.91
2093	CG2	THR			55.854		101.579		56.07
2094	С	THR			57.153	-11.402	99.182	1.00	55.32
2095	0	THR				-11.139	98.285		55.18
2096	N	GLU				-12.330	99.008		52.87
2097	CA	GLU				-13.077	97.771		48.83
2098	СВ	GLU			59.550		97.546	1.00	50.19
2099	CG	GLU			59.720	-14.650	96.488	1.00	49.52
2100	CD	GLU	В	607	59.828	-14.069	95.132	1.00	53.13

FIGURE 1

Amino acid sequence for full length human wild type EPHA2 [SEQ ID NO: 1] (Residues 596-900 are underlined)

MELQAARACFALLWGCALAAAAAAQGKEVVLLDFAAAGGELGWLTHPYGK	50
GWDLMQNIMNDMPIYMYSVCNVMSGDQDNWLRTNWVYRGEAERNNFELNF	100
TVRDCNSFPGGASSCKETFNLYYAESDLDYGTNFQKRLFTKIDTIAPDEI	150
TVSSDFEARHVKLNVEERSVGPLTRKGFYLAFQDIGACVALLSVRVYYKK	200
CPELLQGLAHFPETIAGSDAPSLATVAGTCVDHAVVPPGGEEPRMHCAVD	250
GEWLVPIGQCLCQAGYEKVEDACQACSPGFFKFEASESPCLECPEHTLPS	300
PEGATSCECEEGFFRAPQDPASMPCTRPPSAPHYLTAVGMGAKVELRWTP	350
PQDSGGREDIVYSVTCEQCWPESGECGPCEASVRYSEPPHGLTRTSVTVS	400
DLEPHMNYTFTVEARNGVSGLVTSRSFRTASVSINQTEPPKVRLEGRSTT	450
SLSVSWSIPPPQQSRVWKYEVTYRKKGDSNSYNVRRTEGFSVTLDDLAPD	500
TTYLVQVQALTQEGQGAGSKVHEFQTLSPEGSGNLAVIGGVAVGVVLLLV	550
LAGVGFFIHRRRKNQRARQSPEDVYFSKSEQLKPLKTYVDPHTYE <u>DPNQA</u>	600
VLKFTTEIHPSCVTRQKVIGAGEFGEVYKGMLKTSSGKKEVPVAIKTLKA	650
GYTEKQRVDFLGEAGIMGQFSHHNIIRLEGVISKYKPMMIITEYMENGAL	700
DKFLREKDGEFSVLQLVGMLRGIAAGMKYLANMNYVHRDLAARNILVNSN	750
LVCKVSDFGLSRVLEDDPEATYTTSGGKIPIRWTAPEAISYRKFTSASDV	800
WSFGIVMWEVMTYGERPYWELSNHEVMKAINDGFRLPTPMDCPSAIYQLM	850
MQCWQQERARRPKFADIVSILDKLIRAPDSLKTLADFDPRVSIRLPSTSG	900
SEGVPFRTVSEWLESIKMQQYTEHFMAAGYTAIEKVVQMTNDDIKRIGVR	950
I.PGHOKRTAYSI.I.GI.KDOWNTVGI PI	976

FIGURE 1A

Human cDNA sequence encoding residues 596-900 of EPHA2 [SEQ ID NO: 2]

GACCCCAACCAGGCTGTGTTGAAGTTCACTACCGAGATCCATCC	50
TGTCACTCGGCAGAAGGTGATCGGAGCAGGAGAGTTTGGGGAGGTGTACA	100
AGGGCATGCTGAAGACATCCTCGGGGAAGAAGGAGGTGCCGGTGGCCATC	150
AAGACGCTGAAAGCCGGCTACACAGAGAAGCAGCGAGTGGACTTCCTCGG	200
CGAGGCCGGCATCATGGGCCAGTTCAGCCACCACAACATCATCCGCCTAG	250
AGGGCGTCATCTCCAAATACAAGCCCATGATGATCATCACTGAGTACATG	300
GAGAATGGGGCCCTGGACAAGTTCCTTCGGGAGAAGGATGGCGAGTTCAG	350
CGTGCTGCAGCTGGTGGGCATGCTGCGGGGCATCGCAGCTGGCATGAAGT	400
ACCTGGCCAACATGAACTATGTGCACCGTGACCTGGCTGCCCGCAACATC	450
CTCGTCAACAGCAACCTGGTCTGCAAGGTGTCTGACTTTGGCCTGTCCCG	500
CGTGCTGGAGGACGACCCGAGGCCACCTACACCACCAGTGGCGGCAAGA	550
TCCCCATCCGCTGGACCGCCCCGGAGGCCATTTCCTACCGGAAGTTCACC	600
TCTGCCAGCGACGTGTGGAGCTTTGGCATTGTCATGTGGGAGGTGATGAC	650
CTATGGCGAGCGGCCCTACTGGGAGTTGTCCAACCACGAGGTGATGAAAG	700
CCATCAATGATGGCTTCCGGCTCCCCACACCCATGGACTGCCCCTCCGCC	750
ATCTACCAGCTCATGATGCAGTGCTGGCAGCAGGAGCGTGCCCGCCC	800
CAAGTTCGCTGACATCGTCAGCATCCTGGACAAGCTCATTCGTGCCCCTG	850
ACTCCCTCAAGACCCTGGCTGACTTTGACCCCCGCGTGTCTATCCGGCTC	900
CCCAGCACGAGCGGC	915

Amino acid sequence for residues 596-900 of EPHA2 with a cleavable (rTev) N-terminal 6x-histidine tag [SEQ ID NO: 3] (6x-histidine tag and cleavage site are underlined)

MSYYHHHHHHDYDIPTTENLYFQGAMGSDPNQAVLKFTTEIHPSCVTRQK	50
VIGAGEFGEVYKGMLKTSSGKKEVPVAIKTLKAGYTEKQRVDFLGEAGIM	100
GQFSHHNIIRLEGVISKYKPMMIITEYMENGALDKFLREKDGEFSVLQLV	150
GMLRGIAAGMKYLANMNYVHRDLAARNILVNSNLVCKVSDFGLSRVLEDD	200
PEATYTTSGGKIPIRWTAPEAISYRKFTSASDVWSFGIVMWEVMTYGERP	250
YWELSNHEVMKAINDGFRLPTPMDCPSAIYQLMMQCWQQERARRPKFADI	300
VSILDKLIRAPDSLKTLADFDPRVSIRLPSTSG	333

FIGURE 3

LEGEND

Column headings from left to right are (A) 'Atom Number', (B) 'Atom Type', (C) 'Amino Acid', (D) 'Chain Identifier', (E) 'Amino Acid Number' (SEQ ID NO: 1), (F) 'X Coordinate', (G) 'Y Coordinate', (H) 'Z Coordinate', (I) 'Occupancy' (OCC) and (J) 'B factor'.

1 N ALA A 605	A	В	С	D	E	I	?	G	Н	I	J	
2 CA ALA A 605	1	N	ALA	Α	605	47.2	239 45	.529	67.448	1.00	51.83	
3 CB ALA A 605												
4 C ALA A 605												
5 O ALA A 605		С				46.4	133 47	.259	66.307	1.00	51.78	
6 N THR A 606										1.00	52.61	
7 CA THR A 606		N						.048	65.302	1.00	51.19	
8 CB THR A 606								.337	65.564	1.00	49.98	
10 CG2 THR A 606	8	CB						.120	64.454	1.00	48.98	
11 C THR A 606	9	OG1	THR	Α	606	47.5	553 50	.041	64.401	1.00	50.88	
12 O THR A 606	10	CG2	THR	Α	606	45.7	766 51	.541	64.651	1.00	48.25	
13 N GLU A 607	11	С	THR	Α	606	44.2	201 49	.397	65.650	1.00	50.57	
14 CA GLU A 607	12	0	THR	А	606	43.4	187 48	.868	64.787	1.00	51.60	
15 CB GLU A 607	13	N	GLU	A	607	43.6	580 50	.086	66.646	1.00	49.68	
16 CG GLU A 607	14	CA	${\tt GLU}$	Α	607	42.2	264 50	.182	66.717	1.00	47.97	
17 CD GLU A 607 39.394 49.230 68.074 1.00 39.82 18 OE1 GLU A 607 39.796 48.072 68.195 1.00 38.52 19 OE2 GLU A 607 38.260 49.515 67.856 1.00 41.61 20 C GLU A 607 41.841 51.347 65.971 1.00 48.16 21 O GLU A 607 42.392 52.398 66.162 1.00 48.74 22 N ILE A 608 40.955 51.146 64.963 1.00 50.14 23 CA ILE A 608 40.531 52.309 64.228 1.00 49.42 24 CB ILE A 608 41.128 52.517 62.742 1.00 51.19 25 CG1 ILE A 608 40.066 52.886 61.752 1.00 49.45 26 CD1 ILE A 608 39.259 51.726 61.615 1.00 60.72 27 CG2 ILE A 608 42.168 51.494 62.300 1.00 47.67 28 C ILE A 608 39.135 52.787 64.481 1.00 51.43 29 O ILE A 608 38.254 52.049 64.879 1.00 51.22 30 N HIS A 609 38.983 54.090 64.361 1.00 53.40 31 CA HIS A 609 37.727 54.745 64.674 1.00 55.30 32 CB HIS A 609 37.938 56.203 65.196 1.00 57.26	15	CB	GLU	А	607	41.7	796 50	.123	68.130	1.00	47.41	
18 OE1 GLU A 607 39.796 48.072 68.195 1.00 38.52 19 OE2 GLU A 607 38.260 49.515 67.856 1.00 41.61 20 C GLU A 607 41.841 51.347 65.971 1.00 48.16 21 O GLU A 607 42.392 52.398 66.162 1.00 48.74 22 N ILE A 608 40.955 51.146 64.963 1.00 50.14 23 CA ILE A 608 40.531 52.309 64.228 1.00 49.42 24 CB ILE A 608 41.128 52.517 62.742 1.00 51.19 25 CG1 ILE A 608 40.066 52.886 61.752 1.00 49.45 26 CD1 ILE A 608 39.259 51.726 61.615 1.00 60.72 27 CG2 ILE A 608 42.168 51.494 62.300 1.00 47.67 28 C ILE A 608 39.135 52.787 64.481 1.00 51.43 29 O ILE A 608 38.254 52.049 64.879 1.00 51.22 30 N HIS A 609 38.983 54.090 64.361 1.00 53.40 31 CA HIS A 609 37.727 54.745 64.674 1.00 55.30 32 CB HIS A 609 37.938 56.203 65.196 1.00 57.26	16	CG	GLU	Α	607	40.3	323 50	.414	68.279	1.00	50.07	
19 OE2 GLU A 607 38.260 49.515 67.856 1.00 41.61 20 C GLU A 607 41.841 51.347 65.971 1.00 48.16 21 O GLU A 607 42.392 52.398 66.162 1.00 48.74 22 N ILE A 608 40.955 51.146 64.963 1.00 50.14 23 CA ILE A 608 40.531 52.309 64.228 1.00 49.42 24 CB ILE A 608 41.128 52.517 62.742 1.00 51.19 25 CG1 ILE A 608 40.066 52.886 61.752 1.00 49.45 26 CD1 ILE A 608 39.259 51.726 61.615 1.00 60.72 27 CG2 ILE A 608 42.168 51.494 62.300 1.00 47.67 28 C ILE A 608 39.135 52.787 64.481 1.00 51.43 29 O ILE A 608 38.254 52.049 64.879 1.00 51.22 30 N HIS A 609 38.983 54.090 64.361 1.00 53.40 31 CA HIS A 609 37.727 54.745 64.674 1.00 55.30 32 CB HIS A 609 37.938 56.203 65.196 1.00 57.26	17	CD	GLU	Α	607			.230				
20 C GLU A 607 41.841 51.347 65.971 1.00 48.16 21 O GLU A 607 42.392 52.398 66.162 1.00 48.74 22 N ILE A 608 40.955 51.146 64.963 1.00 50.14 23 CA ILE A 608 40.531 52.309 64.228 1.00 49.42 24 CB ILE A 608 41.128 52.517 62.742 1.00 51.19 25 CG1 ILE A 608 40.066 52.886 61.752 1.00 49.45 26 CD1 ILE A 608 39.259 51.726 61.615 1.00 60.72 27 CG2 ILE A 608 42.168 51.494 62.300 1.00 47.67 28 C ILE A 608 39.135 52.787 64.481 1.00 51.43 29 O ILE A 608 38.254 52.049 64.879 1.00 51.22 30 N HIS A 609 38.983 54.090 64.361 1.00 53.40 31 CA HIS A 609 37.727 54.745 64.674 1.00 55.30 32 CB HIS A 609 37.938 56.203 65.196 1.00 57.26	18	OE1	GLU	Α	607	39.7	796 48	.072	68.195			
21 O GLU A 607 42.392 52.398 66.162 1.00 48.74 22 N ILE A 608 40.955 51.146 64.963 1.00 50.14 23 CA ILE A 608 40.531 52.309 64.228 1.00 49.42 24 CB ILE A 608 41.128 52.517 62.742 1.00 51.19 25 CG1 ILE A 608 40.066 52.886 61.752 1.00 49.45 26 CD1 ILE A 608 39.259 51.726 61.615 1.00 60.72 27 CG2 ILE A 608 42.168 51.494 62.300 1.00 47.67 28 C ILE A 608 39.135 52.787 64.481 1.00 51.43 29 O ILE A 608 38.254 52.049 64.879 1.00 51.22 30 N HIS A 609 37.727 54.745 64.674 1.00 55.30 31 CA HIS A 609 37.938 56.203 65.196 1.00 57.26	19		GLU	A	607	38.2						
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32 CB HIS A 609 37.938 56.203 65.196 1.00 57.26												
33 CG HIS A 609 36.715 56.776 65.635 1.00 60.02												
34 ND1 HIS A 609 36.486 56.686 67.186 1.00 62.57												
34 ND1 HIS A 609 36.486 56.686 67.186 1.00 62.57 35 CE1 HIS A 609 35.313 57.221 67.471 1.00 62.48												
36 NE2 HIS A 609 34.764 57.635 66.348 1.00 63.53												
37 CD2 HIS A 609 35.606 57.345 65.301 1.00 62.09												
38 C HIS A 609 36.701 54.718 63.557 1.00 53.34												
39 O HIS A 609 36.943 55.109 62.474 1.00 55.03												٠,
40 N PRO A 610 35.517 54.263 63.854 1.00 52.90												.:'
41 CA PRO A 610 34.533 54.113 62.805 1.00 53.20												
42 CB PRO A 610 33.246 53.864 63.591 1.00 52.67												
43 CG PRO A 610 33.753 53.087 64.713 1.00 50.94												

FIGURE 3A

A	В	С	D	E	F	G	Н	I	J
44	CD	PRO	Α	610	35.069	53.682	65.133	1.00	52.08
45	С	PRO	A	610	34.421	55.273	61.903	1.00	52.69
46	0	PRO	Α	610	33.935	55.146	60.793	1.00	55.21
47	N	SER	Α	611	34.789	56.418	62.391	1.00	52.17
48	CA	SER	Α	611	34.546	57.584	61.639	1.00	52.33
49	CB	SER	Α	611	34.694	58.833	62.562	1.00	54.93
50	OG	SER	Α	611	35.822	58.723	63.443	1.00	49.81
51	Ç	SER	А	611	35.579	57.611	60.552	1.00	52.77
52	0	SER	Α	611	35.394	58.256	59.545	1.00	54.01
53	N	CYS	Α	612	36.679	56.915	60.701	1.00	49.87
54	CA	CYS	Α	612	37.633	57.083	59.642		51.06
55	CB	CYS	A	612	39.044	56.889	60.169		50.65
56	SG	CYS	Α	612	39.193	57.805	61.702		55.75
57	C	CYS			37.445	56.214	58.426		49.07
58	0	CYS			38.215	56.286	57.479		48.12
59	N	VAL			36.470	55.349	58.497		49.20
60	CA	VAL			36.329	54.361	57.471		48.42
61	CB	VAL			36.130	52.976	58.087		49.58
62	CG1	VAL			35.493	52.026	57.030		46.32
63	CG2	VAL			37.477	52.423	58.651		46.61
64	С	VAL			35.039	54.652	56.779		47.49
65	0	VAL			34.080	55.078	57.401		46.54
66	N	THR			34.976	54.426	55.496		46.87
67	CA	THR			33.674	54.449	54.961		47.76
68	CB	THR			33.230	55.839	54.547		48.10
69	OG1	THR			32.501	55.759	53.312		53.74
70	CG2	THR			34.430	56.804	54.383		48.56
71	C	THR			33.479	53.362 53.317	53.956 52.971		47.36 49.44
72 73	O N	THR ARG			34.145 32.519	52.496	54.192		46.37
73	N				32.319	51.360	53.352		44.80
74 75	CA CB	ARG ARG			31.323	50.464	53.993		43.89
76	CG	ARG			31.817	49.366	54.921		44.82
77	CD	ARG			30.699	48.434	55.297		45.58
78	NE	ARG			29.827	49.226	56.142		49.04
79	CZ	ARG			29.151	48.769	57.151		51.81
80		ARG			29.164	47.437	57.427		50.76
81		ARG			28.473	49.652	57.883		51.85
82	C	ARG			31.694	51.886	52.150		45.54
83	Ō	ARG			30.737	52.603	52.357		47.25
84	N	GLN			32.035	51.399	50.944		45.88
85	CA	GLN			31.366		49.681		46.97
86	CB	GLN			32.323	52.657	48.734	1.00	47.24
87	CG	GLN			33.258	53.608	49.475	1.00	49.82
88	CD	GLN			34.200	54.437	48.588	1.00	55.54
89		GLN			35.203	53.909	48.073		56.72
90	NE2	GLN			33.889	55.770	48.428	1.00	56.51
91	C	GLN			30.597	50.752	48.848	1.00	46.63
92	Ο.	GLN	Α	616	29.448	50.970	48.361	1.00	48.68
93	N	LYS			31.167	49.598	48.678	1.00	44.77
94	CA	LYS	Α	617	30.497	48.628	47.857	1.00	44.21
95	CB	LYS	Α	617	30.835	48.787	46.331	1.00	44.70

FIGURE 3B

A	В	С	D	E	F	G	Н	I	J
96	CG	LYS	Α	617	32.399	48.959	45.944	1.00	48.09
97	CD			617	32.768	48.759	44.391		58.41
98	CE			617	34.285	49.300	44.085	1.00	60.72
99	NZ			617	35.073	48.944	42.813	1.00	59.09
100	С			617	31.019	47.331	48.370	1.00	43.38
101	0	LYS	Α	617	32.139	47.297	48.834	1.00	42.92
102	N			618	30.126	46.333	48.379	1.00	42.86
103	CA	VAL	Α	618	30.376	44.945	48.657	1.00	41.23
104	CB	VAL	Α	618	29.070	44.146	48.522	1.00	39.95
105	CG1	VAL	Α	618	29.426	42.622	48.582	1.00	40.13
106	CG2	VAL	Α	618	28.147	44.503	49.610	1.00	42.60
107	C	VAL	Α	618	31.203	44.381	47.543		40.46
108	0	VAL	Α	618	30.854	44.667	46.392	1.00	42.70
109	N	ILE	Α	619	32.237	43.567	47.809		37.69
110	CA	ILE	Α	619	33.059	43.022	46.731	1.00	33.98
111	CB	ILE	Α	619	34.521	43.786	46.495		36.65
112	CG1	ILE	Α	619	35.584	43.320	47.540		31.94
113	CD1	ILE	Α	619	36.383	44.380	48.493		29.73
114	CG2	ILE	Α	619	34.380	45.336	46.302		31.41
115	C			619	33.357	41.588	46.995		33.91
116	0			619	34.185	41.024	46.280		35.83
117	N			620	32.752	40.970	47.989		32.82
118	CA			620	33.039	39.577	48.271		32.89
119	С	GLY			32.373	39.194	49.553		32.89
120	0			620	31.714	39.949	50.177		30.70
121	N			621	32.511	37.954	49.897		34.15
122	CA	ALA			31.818	37.384	51.019		35.78
123	CB	ALA			30.777	36.453	50.533		35.84
124	C	ALA			32.833	36.551	51.687		37.56
125	0	ALA			33.491	35.782	51.007		39.38
126	N			622	33.026	36.691	52.986		38.91
127	CA			622	34.006 33.398	35.848 34.928	53.611 54.575		38.65 39.55
128	C	GLY		622	33.396	34.920	54.575		36.11
129	O N	GLU			34.293	34.225	55.272		41.01
130 131	N CA			623	33.843	33.363	56.342		41.61
132	CB	GLU			35.046	32.793	57.068		43.27
133	CG			623	34.682				50.78
134	CD			623	35.838	31.063	58.780		65.56
135		GLU			36.962				64.79
136				623	35.592				72.34
137	C			623	32.965				40.39
138	Ō				32.055	33.457	57.987		38.12
139	N			624	33.265	35.347	57.758		37.75
140	CA			624	32.522	35.965	58.889		36.41
141	CB			624	33.506	36.538	59.933		37.60
142	CG			624	34.593	35.546	60.354		34.22
143		PHE			34.285	34.584	61.169		32.75
144	CE1			624	35.256	33.643			42.16
145	CZ			624	36.568				37.78
146				624	36.866		60.168		37.66
147				624	35.861	35.571	59.805		37.30

FIGURE 3C

A	В	С	D	E	F	G	Н	I	J
148	С	PHE	Α	624	31.569	37.066	58.437	1.00	35.68
149	Ō			624	30.875	37.739	59.261	1.00	36.44
150	N			625	31.557	37.336	57.140	1.00	35.15
151	CA	GLY	Α	625	30.731	38.445	56.714	1.00	32.08
152	C	GLY	Α	625	31.164	39.011	55.423	1.00	32.29
153	0	GLY	A	625	32.177	38.633	54.858	1.00	32.00
154	N	GLU	Α	626	30.422	39.990	54.988	1.00	33.82
155	CA	GLU	A	626	30.710	40.519	53.695	1.00	37.80
156	CB	GLU	Α	626	29.534	41.289	53.103	1.00	36.83
157	CG	GLU	А	626	28.396	40.298	52.839	1.00	42.38
158	CD	GLU	Α	626	27.343	40.941	51.992		45.04
159	OE1	GLU			27.289	40.680	50.777		47.93
160	OE2	GLU			26.632	41.773	52.553		43.41
161	C			626	31.896	41.377	53.719		37.16
162	0			626	32.262	41.878	54.803		35.84
163	N			627	32.477	41.552	52.508		35.91
164	CA			627	33.711	42.268	52.392		34.05
165	CB			627	34.839	41.340	51.861		36.58
166	CG1	VAL			36.210	42.135	51.691		30.17
167	CG2	VAL			34.986	40.244	52.740		33.27
168	C			627	33.388	43.380	51.461		34.18
169	0			627	32.633	43.157	50.568 51.680		31.95
170	N			628	33.990	44.575	50.948		33.62 33.35
171	CA			628 628	33.618 32.892	45.746 46.766	51.894		35.70
172 173	CB CG			628	31.519	46.700	52.411		35.23
174	CD1			628	31.344	45.529	53.497		34.62
175	CE1			628	30.088	45.215	53.976		36.28
176	CZ			628	28.935	45.759	53.348		39.83
177	OH			628	27.634	45.479	53.748		41.33
178	CE2			628	29.080	46.582	52.266		43.12
179	CD2			628	30.397	46.941	51.826		40.98
180	C			628	34.890	46.407	50.597	1.00	33.72
181	0	TYR	Α	628	35.938	46.184	51.223	1.00	35.69
182	N	LYS	Α	629	34.749	47.365	49.743	1.00	33.77
183	CA	LYS	Α	629	35.792	48.236	49.369	1.00	36.45
184	CB	LYS	Α	629	35.613	48.688	47.939	1.00	36.34
185	CG	LYS	Α	629	36.692	49.598	47.624		41.68
186	CD	LYS	Α	629	36.232	50.858	47.072		45.46
187	CE	LYS	Α	629	37.426	51.809	46.890		51.36
188	NZ	LYS	Α	629	36.962				49.95
189	C			629	35.440	49.455	50.046		37.55
190	0			629	34.298	49.740	50.227		37.87
191	N	GLY			36.415	50.286	50.355		41.21
192	CA	GLY			36.010	51.559	50.912		42.33
193	C	GLY			37.204	52.450	51.067		44.89
194	0	GLY			38.205	52.287	50.392		45.71
195	N	MET			37.086	53.363	52.008		46.92
196	CA	MET			38.014	54.443	52.136		48.84
197	CB	MET			37.379		51.608		49.65
198	CG			631	37.177		50.070		51.92
199	SD	WE.I.	A	631	38.727	55.249	49.171	1.00	57.95

FIGURE 3D

A	В	C	D	E		F	G	Н	I	J
200	CE	MET				39.478	56.799	48.727		56.76
201	C	MET				38.379	54.619	53.587		49:23
202	0	MET				37.493	54.616	54.462		47.16
203	N			632		39.696	54.667	53.828		47.01
204	CA			632		40.144	54.951	55.148		48.50
205	CB			632		41.204	53.954	55.531		46.95
206	CG	LEU				41.924	54.217	56.805		47.11
207		LEU				40.936	53.899	57.902		45.89
208	CD2	LEU				43.172	53.311	-		47.90
209	C	LEU				40.680	56.425	55.221		50.08
210	0	LEU				41.388	56.932	54.323		47.85
211	N	ALA				40.279	57.138	56.256		52.44
212	CA	ALA				40.873	58.465	56.388		56.35
213	СВ	ALA				39.848	59.562	56.836		55.50
214	C	ALA				41.842	58.189	57.445		56.34
215	0	ALA				41.406	57.920	58.493		58.62
216	N	ALA				43.136	58.194	57.224		57.84
217	CA	ALA				43.920	57.980	58.415		61.35
218	CB	ALA				45.364	57.774	58.115		62.22
219	C	ALA				43.771	59.263	59.222		62.67
220	0			634		44.422	60.208	58.850		64.38
221	N			638		43.383	64.048	56.993	1.00	
222	CA	ALA				44.752	64.060	56.359		79.12
223	CB	ALA				45.788	63.305	57.237		78.95
224	C	ALA				44.822	63.605	54.872		79.32
225	0	ALA				45.141	64.402	54.006	1.00	
226	N	ALA				44.531	62.334	54.589	1.00	78.59
227	CA	ALA				44.620	61.761	53.238	1.00	77.38
228	CB	ALA				46.119	61.531	52.875	1.00	
229	C	ALA				43.843	60.408	53.247	1.00	75.52
230	0			639		44.050	59.569	54.155		75.87
231	N			640		42.935	60.248	52.273	1.00	71.51
232	CA	GLU				41.968	59.139	52.171		66.84
233	CB	GLU				40.701	59.599	51.433		66.51
234	CG	GLU				39.483	58.732	51.713		68.84
235	CD	GLU				38.106	59.433	51.585	1.00	70.86
236	OE1	GLU				37.834	60.052	50.511	1.00	71.60
237		GLU			•	37.274		52.561		70.47
238	C	GLU				42.571	58.052	51.379		63.66
239	0			640		43.179	58.300	50.363		64.69
240	N	VAL				42.394	56.821	51.807		60.16
241	CA	VAL				43.028	55.721	51.100		55.19
242	CB	VAL				44.352	55.368	51.777		54.62
243	CG1	VAL				44.223	54.272	52.749		50.91
244	CG2	VAL				45.363	55.043	50.767		56.67
245	С	VAL				42.102	54.570	50.931		52.53
246	0			641		41.378	54.194	51.812		55.11
247	N			642		42.105	53.989	49.767		51.34
248	CA	PRO				41.271	52.776	49.477		47.14
249	CB	PRO				41.664	52.399	48.064		47.64
250	CG	PRO						47.544		50.33
251	CD	PRO	A	642		42.943	54.475	48.637	1.00	50.56

FIGURE 3E

A	В	С	D	E	F	G	Н	I	J
252	С	PRO	А	642	41.625	51.589	50.367	1.00	45.19
253	0			642	42.816	51.373	50.765		44.61
254	N			643	40.636	50.779	50.710		40.92
255	CA	VAL			40.925	49.716	51.646	1.00	
256	CB			643	40.652	50.209	53.117		37.96
257	CG1	VAL			41.889	50.869	53.733		39.75
258	CG2	VAL			39.377	51.186	53.225		32.90
259	C			643	39.921	48.664	51.373		36.92
260	0			643	38.827	48.941	50.848		38.74
261	N			644	40.226	47.464	51.769		34.90
262	CA			644	39.217	46.411	51.722		34.08
263	CB			644	39.858	45.092	51.412		31.97
264	C			644	38.726	46.373	53.179		35.58
265	0			644	39.526	46.712	54.096		30.86
						45.968	53.393		36.25
266	N			645	37.443		54.744		34.97
267	CA			645 645	36.922	45.950	54.744		35.85
268	CB				35.932	47.080			
269	CG1			645	36.577	48.336	54.488		37.94
270	CD1			645	35.489	49.480	54.224		39.26
271	CG2			645	35.314	47.127	56.304		32.71
272	C			645	36.201	44.682	55.066		33.98
273	0			645	35.113	44.491	54.584	1.00	
274	N			646	36.714	43.846	55.922		34.87
275	CA	LYS			36.008	42.632	56.289		38.18
276	CB			646	37.040	41.499	56.633		39.75
277	CG	LYS			37.905	41.096	55.427		44.65
278	CD	LYS			38.718	39.873	55.721		47.74
279	CE	LYS			38.775	38.957	54.557		56.44
280	NZ	LYS			40.016	39.325	53.698		67.82
281	C	LYS			35.078	42.871	57.482	1.00	
282	0	LYS			35.524	43.217	58.526		39.11
283	N	THR			33.779	42.703	57.344		38.53
284	CA			647	32.898	42.869	58.518		35.17
285	CB	THR			31.620	43.563	58.086		35.95
286	OG1	THR			30.886	42.779	57.136		31.75
287	CG2	THR			31.977	44.751	57.224		26.19
288	C	THR			32.581	41.580	59.205		35.41
289	0	THR			32.741	40.482	58.693		36.20
290	N	LEU			32.208	41.704	60.429		35.38
291	CA			648	31.915		61.187		37.01
292	CB	LEU			32.612	40.708	62.523		36.29
293	CG	LEU			32.176	39.634	63.510		34.38
294	CD1	LEU			32.349	38.265	63.066		33.21
295	CD2	LEU			32.938	39.707	64.670		38.96
296	C	LEU			30.383	40.645	61.334		39.65
297	0	LEU			29.873	41.630	61.869		41.32
298	N	LYS	Α	649	29.631	39.670	60.813		39.93
299	CA	LYS			28.175	39.764	60.832		38.04
300	CB	LYS			27.610	38.564	60.128		38.58
301	CG	LYS			27.766	37.309	60.890		38.14
302	CD	LYS			27.679		59.889		35.47
303	CE	LYS	А	649	27.535	34.883	60.524	1.00	35.35

FIGURE 3F

A	В	С	D	E		F		G		Н	I	J
304	NZ	LYS	Α	649	27	7.499	33.	710	59	9.600	1.00	36.16
305	C	LYS			27	7.630	39.	998	62	2.226	1.00	38.13
306	0	LYS			28	3.217	39.	517	63	3.181	1.00	38.78
307	N	ALA	Α	650	26	5.642	40.	900	62	2.370	1.00	38.37
308	CA	ALA	Α	650	26	5.009	41.	267	63	3.688	1.00	38.30
309	CB	ALA	Α	650	24	1.721	41.	954	63	3.443	1.00	37.99
310	C	ALA	Α	650	25	5.680	39.	928	64	1.183	1.00	38.32
311	0	ALA	Α	650	25	5.410	39.	138	63	3.320	1.00	40.75
312	N	GLY	Α	651	25	5.632	39.	493	65	.416	1.00	35.55
313	CA	GLY	А	651	25	5.195	38.	071	65	5.179		36.67
314	C	GLY	Α	651	26	5.171	36.	916	65	5.234	1.00	33.22
315	0	GLY	Α	651	25	5.899		767		5.646		30.70
316	N	TYR	Α	652	27	7.390	37.	294	65	5.039		34.28
317	CA	TYR	Α	652	28	3.455	36.	416	65	5.446		36.25
318	CB	TYR	Α	652	29	9.684	37.	205		5.494		38.05
319	CG	TYR			29	9.668		292		5.484		38.76
320	CD1	TYR			3 (0.221	38.	086		7.745		36.74
321	CE1	TYR			3 (0.242		091		3.684		34.51
322	CZ	TYR				9.778		325		3.329		40.27
323	OH			652	29	9.893		245		9.291		42.40
324	CE2	TYR				9.178		584		7.038		34.15
325	CD2	TYR				9.169		556		5.141		38.47
326	C			652		3.386		850		5.803		35.31
327	0	TYR				7.919		531		7.696		34.45
328	N	THR				3.961		652		5.947		35.94
329	CA	THR				9.209		999		3.234		36.94
330	CB			653		9.248		522		3.183		37.69
331	OG1			653		0.427		201		7.433		40.83
332	CG2	THR				3.007		792		7.363		32.24
333	C			653		0.595		418		3.718		37.14
334	0			653		1.347		985		3.015		37.03
335	N			654		0.831		210		9.998		37.12
336	CA			654		2.094		484		0.674		37.20
337	CB			654		2.074		802		2.025		34.84 44.32
338	CG			654		3.380		188		2.705		44.32
339	CD OE1			654		3.571 2.591		731		2.609 2.366		54.40
340	OE1	GLU				1.675		206		2.300		46.32
				654		3.316		880		9.890		35.96
342	C			654		1.306		579		9.620		33.58
343	O M					3.161		605		9.577		35.57
344	N CA			655 655		1.030		857		3.747		39.28
345	CB			655		3.532		394		3.482		39.74
346 347	CG			655		1.682		481		3.003		46.57
				655		1.375		446		5.854		53.64
348 349	CD CE			655		5.674		584		5.374		58.92
350	NZ			655		7.147		174		5.350	1.00	
350	C			655		1.326		574		7.379	1.00	
352	0			655		5.481	.32.			7.012		41.81
352	N			656		3.329		111		5.678		35.08
354	CA			656		3.583		809		5.411		36.08
355	CB			656		2.355		070		1.590		32.82
								-	-			

FIGURE 3G

A	В	. C	D	Е	F	G	Н	I	J
356	CG	GLN	A	656	31.709	32.793	64.216	1.00	35.27
357	CD	GLN	Α	656.	30.255	32.982	63.707	1.00	37.96
358	OE1	GLN	A	656	29.471	33.846	64.157	1.00	30.18
359	NE2	GLN	Α	656	29.948	32.217	62.693	1.00	42.57
360	C	GLN	Α	656	34.305	35.111	65.659	1.00	35.54
361	0	GLN	Α	656	35.196	35.485	64.899	1.00	35.47
362	N	ARG	Α	657	33.951	35.722	66.760	1.00	35.39
363	CA	ARG	Α	657	34.557	36.985	67.147	1.00	39.00
364	CB	ARG	Α	657	33.923	37.539	68.413	1.00	37.06
365	CG	ARG	А	657	34.401	38.841	68.811	1.00	40.49
366	CD	ARG	A	657	34.033	39.137	70.269	1.00	41.44
367	NE	ARG	Α	657	34.843	40.262	70.614	1.00	54.97
368	CZ	ARG	Α	657	35.982	40.205	71.383	1.00	54.52
369	NH1	ARG	Α	657	36.451	39.051	71.945	1.00	43.49
370	NH2	ARG	A	657	36.616	41.349	71.556		55.48
371	C	ARG	Α	657	36.017	36.717	67.311	1.00	38.95
372	0	ARG	Α	657	36.826	37.240	66.592	1.00	37.52
373	N	VAL	A	658	36.331	35.771	68.150	1.00	42.72
374	CA	VAL	Α	658	37.722	35.481	68.321	1.00	45.25
3 75	CB	VAL	Α	658	37.957	34.577	69.517	1.00	47.74
376	CG1	VAL	Α	658	39.291	33.787	69.368		48.43
377	CG2	VAL			37.935	35.483	70.791	1.00	49.98
378	C	VAL	А	658	38.449	35.036	67.044	1.00	45.07
379	0	VAL	Α	658	39.466	35.669	66.720	1.00	44.99
380	N	ASP	А	659	37.913	34.045	66.299	1.00	42.92
381	CA	ASP	Α	659	38.561	33.655	65.043		41.99
382	CB	ASP			37.891	32.498	64.307		41.26
383	CG	ASP	Α	659	37.826	31.278	65.1 77		45.94
384	OD1	ASP			37.109	30.301	64.847		46.31
385		ASP			38.451	31.252	66.249		43.77
386	C	ASP			38.683	34.857	64.176		39.97
387	0	ASP			39.687	35.012	63.586	1.00	
388	N			660	37.703	35.756	64.220	1.00	
389	CA			660	37.765	36.881	63.312		39.49
390	CB			660	36.385	37.556	63.203	1.00	
391	CG			660	36.343	38.830	62.388	1.00	33.56
392		PHE			36.342	40.047	62.976	1.00	
393		PHE			36.323		62.257		28.65
394	CZ			660	36.136	41.248	60.858		24.95
395		PHE			36.059	40.060	60.259		28.98
396	CD2			660	36.099		61.088		32.15
397	C			660	38.897	37.885	63.675		39.32
398	0			660	39.584	38.276	62.825		38.41
399	N			661	39.061	38.276	64.928		40.15
400	CA	LEU			40.011	39.306	65.232		42.07
401	CB	LEU			39.711	39.915	66.582		43.38
402	CG			661	38.437	40.774	66.709		43.55
403	CD1	LEU			38.306	41.372	68.133		39.97
404	CD2			661 .	38.580	41.902	65.756		37.68
405	C			661	41.347	38.552	65.294		41.94
406	0			661	42.340	39.129			41.62
407	N	GГY	A	662	41.349	37.252	65.485	1.00	39.75

FIGURE 3H

A	В	C	D	E	F	י	G	Н	I	J
408	CA			662	42.6		36.635	65.570		40.93
409	C			662	43.4		36.757	64.273		43.18
410	0			662	44.5		37.160	64.286		42.86
411	N			663	42.7		36.439	63.154		42.57
412	CA			663	43.3		36.553	61.894		42.39
413	CB			663	42.3		36.281	60.792		44.11
414	CG			663	42.8		36.991	59.480		48.03
415	CD			663	42.3		36.230	58.234		54.58
416	OE1			663	41.2		35.605	58.330		52.44
417	OE2	GLU			43.2		36.292	57.213	1.00	
418	С			663	43.9		37.968	61.741		40.61
419	0			663	45.0		38.192	61.213		37.63
420	N			664	43.2		38.944	62.230		38.99
421	CA			664	43.9		40.237	62.062		40.23
422	CB			664	42.9		41.347	62.358		41.34
423	С			664	45.1		40.278	63.055		39.40
424	0			664	46.1		40.873	62.831		39.10
425	N			665	44.9		39.570	64.138		38.27
426	CA			665	46.0		39.586	65.064		42.63
427	C			665	47.3		39.076	64.355		44.59
428	0			665	48.4		39.610	64.610		45.78
429	N			666	47.2		38.070	63.464		44.36
430	CA			666	48.2	95	37.277	62.941		42.46
431	CB	ILE	A	666	47.6	27	36.023	62.510		44.08
432	CG1	ILE	Α	666	47.2	47	35.276	63.731		42.77
433	CD1	ILE	Α	666	46.3	94	34.096	63.279		43.64
434	CG2			666	48.4		35.006	61.565		42.50
435	C	ILE	Α	666	48.8	346	38.081	61.853		41.32
436	0			666	49.9		38.330	61.798		41.39
437	N			667	47.9		38.726	61.143		41.98
438	CA			667	48.3		39.417	59.971		41.72
439	CB			667	47.C		39.871	59.303		42.41
440	CG			667	47.1		40.885	58.149		41.60
441	SD			667	45.3		40.798	57.345	1.00	
442	CE			667	44.9		39.215	57.870		44.36
443	C			667	49.1		40.575	60.497		42.65
444	0	MET			50.0		41.128	59.816		38.11
445	N	GLY			48.7		40.953	61.734		42.74
446	CA	GLY			49.3		42.203	62.310		42.47
447	C			668	50.8		42.083	62.677		40.74
448	0	GLY			51.5		43.010	62.772		39.44
449	N	GLN			51.2		40.861	62.790		40.10
450	CA	GLN			52.5		40.577	63.149		40.54
451	CB	GLN			52.5		39.193	63.729		39.50
452	CG	GLN			52.0		39.318	65.065	1.00	
453	CD	GLN			51.8		37.999	65.772		53.41
454	OE1	GLN			50.7		37.616	66.048		59.36
455	NE2	GLN			52.9		37.334	66.121		57.56
456	C	GLN			53.4		40.657	61.955		41.95
457	0	GLN			54.6		40.622	62.152		41.00
458	N		•	670	52.9		40.908	60.729		40.25
459	CA	PHE	A	670	53.7	38	40.932	59.578	1.00	38.18

FIGURE 3I

A	В	C	D	E		F	C	3	F	I	I	J
			_								1 00	. 40 10
460	CB	PHE.				3.159			58.5			40.10
461	CG	PHE				2.990			59.1			35.26
462	CD1	PHE				L.962	37.8		58.7			33.32
463	CE1	PHE				L.803			59.2			35.47
464	CZ	PHE				2.720			59.9			36.73
465	CE2	PHE				3.818			60.3			40.51
466	CD2	PHE				3.948			59.8			37.75
467	C	PHE				3.941			58.9			39.07
468	0	PHE				3.038			59.0			37.82
469	N	SER				5.170			58.4			37.93
470	CA	SER				3.327			57.7			39.08
471	CB	SER				5.937			58.5			40.17
472	OG	SER				5.915			57.7			43.39
473	C	SER				5.231			56.4			41.33
474	0	SER				7.490			56.5			38.64
475	N	HIS				5.586			55.2			42.48
476	CA	HIS				5.279			54.0			42.62
477	CB	HIS				5.565	41.3		54.1			42.23
478	CG	HIS				7.524			53.1			47.30
479	ND1	HIS				7.142	40.7		51.8			46.67
480	CE1	HIS				3.240			51.1			45.98
481	NE2	HIS				9.289			51.9			44.11
482	CD2	HIS			58	3.874			53.2			45.01
483	C	HIS				5.513			52.8			42.33
484	0	HIS				1.388			52.7			41.57
485	N (HIS				5.192			51.8			42.80
486	CA	HIS				5.610			50.5			42.36
487	CB	HIS				5.722			49.5			38.97
488	CG	HIS				5.262			48.2			46.80
489	ND1					5.503			48.2			49.74
490		HIS				5.348			46.9			43.86
491	NE2	HIS				5.959			46.1			43.54
492	CD2	HIS				5.496			46.9			42.26
493	C	HIS				1.523	43.1		49.8			40.55
494	0	HIS				3.543	43.6		49.3			42.61
495	N	ASN				1.764			50.0			36.25
496	CA	ASN				1.035	40.8		49.3		1.00	
497	CB	ASN				5.074						39.80
498	CG	ASN				5.870	40.5		47.6			36.97
499		ASN				5.321			46.5			35.65
500		ASN				7.139			47.8			37.21
501	C	ASN				3.281	40.1		50.4			38.05
502	0	ASN				3.058	38.9		50.2			37.79
503	N	ILE				2.996	40.8		51.5			38.03
504	CA	ILE				2.081	40.3		52.6			36.57
505	CB	ILE				2.790	40.1		53.9			36.46
506	CG1	ILE				3.903			53.6			33.71
507	CD1	ILE				3.464			53.4			35.15
508	CG2	ILE				L.921	39.4		54.9			31.06
509	С	ILE				979			52.7			38.05
510	0	ILE				L.256			52.8			35.21
511	N	ILE	A	676	49	724	40.9	902	52.6	61	1.00	37.36

FIGURE 3J

A	В	С	D	E	F	C	3	Н	I	J
512	CA	ILE	Α	676	48.63	L7 41.8	368 52	2.857	1.00	37.03
513	CB			676	47.22			2.874		37.73
514	CG1	ILE			46.73			.432		41.75
515	CD1			676	46.82			.877	1.00	38.59
516	CG2	ILE			46.10			3.361	1.00	39.38
517	C			676	48.79			.162	1.00	35.26
518	0			676	48.9			.242	1.00	
519	N			677	48.68			.025	•	34.27
520	CA	ARG			48.9			.101	1.00	36.19
521	CB	ARG			49.49	94 46.0		.510		36.64
522	CG	ARG			49.53	36 47.1		5.599		41.64
523	CD	ARG			50.50			.229		47.74
524	NE	ARG			49.82			.572	1.00	53.55
525	CZ	ARG			49.79			.246	1.00	61.80
526	NH1	ARG	Α	677	50.42	25 48.6	510 52	.436	1.00	54.93
527	NH2	ARG	Α	677	49.09	96 50.5	68 52	2.734	1.00	55.75
528	С	ARG			47.6	70 45.1	.63 55	.876	1.00	35.14
529	0	ARG	А	677	46.72	23 45.6	524 55	3.334	1.00	37.56
530	N	LEU	Α	678	47.6		07 57	7.161	1.00	36.98
531	CA	LEU	Α	678	46.5	77 45.3	306 58	3.012	1.00	37.75
532	CB	LEU	Α	678	46.63	36 44.5	33 59	.287	1.00	37.13
533	CG	LEU	Α	678	45.64	44 45.0	03 60	.367	1.00	38.89
534	CD1	LEU	Α	678	44.18	36 44.6	529 59	808.	1.00	40.66
535	CD2	LEU	А	678	45.90	9 44.2	223 61	548	1.00	36.72
536	C	LEU	Α	678	46.59	2 46.7	739 58	3.328	1.00	36.93
537	0	LEU	Α	678	47.50	5 47.2	253 58	8.861	1.00	37.75
538	N	GLU	Α	679	45.58	35 47.4	52 57	7.961	1.00	40.76
539	CA	GLU	Α	679	45.58	33 48.8	329 58	3.351	1.00	41.67
540	CB	GLU	Α	679	44.59	96 49.5	592 57	7.532	1.00	42.01
541	CG	GLU	Α	679	45.04	15 49.7	720 56	5.088	1.00	43.00
542	CD	GLU	Α	679	46.20	08 50.6	542 55	.968	1.00	54.85
543	OE1	GLU	Α	679	47.05	55 50.2	299 55	.162	1.00	60.51
544	OE2	GLU	Α	679	46.32	21 51.6	78 56	6.698	1.00	58.17
545	C	GLU	А	679	45.18	32 48.9	39 59	817	1.00	43.77
546	0	GLU	A	679	45.57	79 49.9	921 60	.483	1.00	45.58
547	N	GLY			44.38	33 47.9		.317	1.00	43.57
548	CA	GLY			43.77			635		43.39
549	C	GLY	Α	680	42.42	28 47.4	36 61	.718	1.00	43.49
550	0	GLY	Α	680	41.87			730		43.61
551	N	VAL	Α	681	41.91	L7 47.3	300 62	2.921		43.77
552	CA	VAL			40.63			3.148		45.21
553	CB	VAL	Α	681	40.73	39 45.5		.095		44.87
554	CG1	VAL			41.83			.645		46.36
555	CG2	VAL			41.16			.458		48.19
556	С	VAL			39.71			8.826		47.24
557	0	VAL			40.14			.420		49.54
558	N	ILE			38.44			8.827		47.38
559	CA	ILE			37.41			.569		48.87
560	CB	ILE			36.37			3.710		48.22
561	CG1	ILE			36.95			2.995		48.43
562	CD1			682	35.99			2.288		44.35
563	CG2	ILE	Α	682	35.35	0 49.0	079 64	.642	1.00	51.05

FIGURE 3K

A	В	C	D	E	1	F	G	Н	I	J
	_		_		26.1		46 000	CE 42	0 1 00	40.00
564	C			682	36.		46.983	65.43		49.28
565	0			682	36.		46.091	64.92		47.34
566	N			683	37.		47.028	66.72		49.45
567	CA			683	36.		46.043	67.62		52.94
568	CB			683	37.		45.283	68.23		52.37
569	OG			683	38.		46.148	69.03		57.12
570	C			683	35.8		46.665	68.79		55.66
571	0			683	35.		45.961	69.63		56.40
572	N			684	35.8		47.987	68.88		57.01
573	CA			684	35.3		48.589	70.04		57.46
574	CB			684	36.		49.729	70.59		56.07
575	CG			684	37.	282	49.187	71.56		58.30
576	CD	LYS	Α	684	38.0	630	49.925	71.44		58.07
577	CE	LYS	Α	684	38.	562	51.505	71.95		65.46
578	NZ	LYS	Α	684	39.		52.366	71.88		62.96
579	C	LYS	Α	684	33.	821	48.865	69.72	7 1.00	57.78
580	0	LYS	Α	684	32.	999	48.795	70.58	0 1.00	58.15
581	N	TYR	Α	685	33.4	467	48.977	68.46		58.96
582	CA	TYR	Α	685	32.	075	49.289	68.08	6 1.00	59.96
583	CB	TYR	Α	685	31.	994	50.682	67.47	3 1.00	60.66
584	CG	TYR	Α	685	32.	713	51.794	68.19	5 1.00	63.95
585	CD1	TYR	Α	685	32.	081	53.033	68.44	4 1.00	68.40
586	CE1	TYR	Α	685	32.	793	54.105	69.05	6 1.00	72.55
587	CZ	TYR	Α	685	34.	165	53.916	69.40	1 1.00	73.82
588	OH	TYR	Α	685	34.	955	54.898	70.02	3 1.00	70.57
589	CE2	TYR	Α	685	34.	766	52.684	69.11	6 1.00	70.32
590	CD2	TYR	Α	685	34.	035	51.660	68.52	3 1.00	65.77
591	С	TYR	Α	685	31.4	407	48.309	67.09	0 1.00	60.40
592	0	TYR	Α	685	32.	026	47.310	66.71	3 1.00	61.88
593	N	LYS	Α	686	30.	162	48.569	66.64	9 1.00	59.90
594	CA	LYS	Α	686	29.	579	47.680	65.65	6 1.00	58.82
595	CB	LYS	Α	686	28.4	498	46.716	66.02	4 1.00	59.93
596	CG	LYS	Α	686	29.	096	45.424	66.53	0 1.00	59.37
597	CD	LYS	Α	686	29.	072	45.326	68.04	0 1.00	64.32
598	CE	LYS	Α	686	30.3	146	46.244	68.67	6 1.00	67.97
599	NZ	LYS	Α	686	30.	718	45.703	69.95	7 1.00	66.41
600	C	LYS	A	686	29.	658	47.859	64.24	2 1.00	59.00
601	0	LYS	Α	686	29.4	403	48.925	63.67	3 1.00	61.49
602	N	PRO	Α	687	29.4	432	46.717	63.73	5 1.00	56.91
603	CA			687	30.	101	45.699	63.00	6 1.00	53.48
604	CB	PRO	Α	687	29.8		46.015	61.54	6 1.00	55.46
605	CG	PRO	Α	687	28.	763	47.004	61.47	0 1.00	56.97
606	CD			687	28.		47.506	62.79		57.11
607	С			687	31.5		45.851	63.40		50.95
608	0			687	32.:		46.919	63.37		49.51
609	N	MET			32.3		44.784	63.86		48.57
610	CA	MET			33.6		44.783	63.90		45.58
611	СВ	MET			34.		43.690	64.78		44.26
612	CG	MET			33.3		43.867	66.12		46.14
613	SD	MET			34.:		42.726	67.12		50.45
614	CE	MET			32.9		42.348			55.70
615	C	MET			34.		44.576	62.44		45.64
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FIGURE 3L

Α	В	С	D	E		F		G		Н	I	J
616	0	MET	А	688	3	3.364	4	3.928	61	.647	1.00	43.85
617	N	MET	Α	689	3	5.223	4	5.158	62	.136	1.00	44.48
618	CA	MET	A	689	3	5.872	4	5.203	60	.853	1.00	41.56
619	CB	MET	Α	689	3	5.682	4	6.594	60	.344	1.00	40.68
620	CG	MET	Α	689	3	4.291	4	6.942	60	.319	1.00	37.62
621	SD	MET	Α	689	3	3.939	4	8.310	59	.192	1.00	42.01
622	CE	MET	Α	689	3	4.300	4	9.294	60	.146	1.00	46.45
623	C	MET	Α	689	3	7.362	4	4.919	60	.908	1.00	41.69
624	0	MET	A	689	3	7.977	4	5.178	61	.897	1.00	39.55
625	N	ILE	Α	690	3	7.940	4	4.373	59	.830	1.00	40.03
626	CA	ILE	A	690	3	9.410	4	4.156		.726	1.00	38.46
627	CB			690		9.650		2.717		.574	1.00	38.25
628	CG1	ILE	Α	690	3	9.323		2.011		.848	1.00	33.60
629	CD1			690		9.562		0.492		.720	1.00	36.97
630	CG2			690		1.038		2.467		.271	1.00	40.53
631	C			690		9.644		4.923		.495	1.00	38.31
632	0	ILE		690		8.862		4.775		.519	1.00	38.24
633	N			691		0.509		5.952		.568	1.00	39.22
634	CA	ILE		691		0.764		6.894		.444	1.00	36.53
635	CB			691		0.907		8.317		.943	1.00	37.55
636	CG1			691		9.876		8.734		.047	1.00	39.31
637	CD1			691		8.393		8.990		.541	1.00	32.39
638	CG2			691		0.907		9.256		.831	1.00	37.29
639	C			691		2.158		6.590		.770	1.00	38.01
640	0			691		3.218		6.620		.463	1.00	38.01
641	N	THR				2.182		6.381		.445	1.00	37.20
642	CA	THR				3.445		6.080		.734	1.00	36.47
643	CB	THR				3.566		4.593		.387	1.00	35.20
644	OG1	THR				2.564		4.283		.451	1.00	35.83
645	CG2	THR				3.156		3.824		.543	1.00	30.57
646	C	THR				3.683		6.861		.537	1.00	36.06
647	0	THR				2.841		7.599		.075	1.00	37.50
648	N	GLU				4.893		6.762		.018	1.00	36.84
649	CA	GLU				5.200		7.581		.862 .456	1.00	34.75 34.83
650	CB	GLU				6.688				.430	1.00	37.28
651 652	CG CD	GLU GLU				7.212 8.611		5.989 5.888		.934	1.00	40.39
653		GLU				9.308		4.958		.275		45.33
654	OE2	GLU				9.039		6.754		.177	1.00	
655	C	GLU				4.262		7.082		.823		35.09
656	0	GLU				3.970		5.920		.773		36.98
657	N	TYR				3.698		7.978		.038		36.62
658	CA	TYR				2.849		7.622		.960		37.31
659	CB	TYR				2.179		8.887		.452		37.54
660	CG	TYR				1.184		8.414		.412		42.14
661	CD1	TYR				1.184		8.943		.116	1.00	
662	CE1	TYR				0.308		8.458		.146		43.19
663	CZ	TYR				9.456		7.373		.442		43.99
664	OH	TYR				8.543		6.885		.453	1.00	
665	CE2	TYR				9.497		6.773		.700	1.00	
666	CD2	TYR				0.400		7.254		.673		43.35
667	C	TYR				3.600		6.896		.705		37.33
557	~	11	- 1	J J I	-		-2		- '			

FIGURE 3M

А	В	C	D	E	F	G	Н	I	J
668	0	TVD	Δ	694	44.550	47.410	47.236	1.00	36.42
669	N			695	43.211	45.693	47.297		36.44
670	CA			695	43.873	45.008	46.147		38.70
671	CB			695	44.266	43.583	46.553		36.76
672	CG			695	45.185	43.564	47.793		36.63
673	SD			695	46.870	44.267	47.620		38.01
674	CE			695	47.436	42.869	46.677		33.07
675	C			695	42.889	44.957	44.909		40.11
676	0			695	42.039	44.111	44.843		42.18
677	N			696	43.005	45.883	43.975		40.26
678	CA			696	42.088	46.032	42.896		41.93
679	CB			696	42.712	46.973	41.893		43.18
680	CG			696	42.480	48.440	42.115		48.76
681	CD			696	41.565	48.937	40.999		58.48
682	OE1	GLU			40.566	48.194	40.663		63.90
683	OE2	GLU			41.916	50.017	40.443		62.65
684	C			696	41.889	44.764	42.103		41.93
685	Ō			696	40.789	44.446	41.706		44.34
686	N			697	42.922	43.979	41.880		39.85
687	CA			697	42.618	42.947	40.921		38.87
688	CB			697	43.808	42.705	39.966	1.00	38.40
689	CG			697	43.812	43.672	38.784	1.00	40.20
690		ASN			44.849	44.178	38.347	1.00	44.17
691	ND2	ASN	Α	697	42.558	43.959	38.269	1.00	45.86
692	C	ASN	Α	697	42.157	41.756	41.647	1.00	37.90
693	0	ASN	Α	697	41.992	40.689	41.026	1.00	39.69
694	N	GLY	Α	698	42.062	41.848	42.992	1.00	33.49
695	CA	GLY	Α	698	41.403	40.701	43.621	1.00	28.87
696	C	GLY	А	698	42.204	39.491	43.680	1.00	29.77
697	0	GLY	Α	698	43.383	39.592	43.682		29.55
698	N	ALA	Α	699	41.559	38.342	43.701	1.00	29.72
699	CA			699	42.186	37.154	43.998	1.00	
700	CB			699	41.204	36.198	44.395	1.00	
701	С			699	42.995	36.675	42.794	1.00	
702	0			699	42.596	36.859	41.676		31.03
703	N			700	44.050	35.887	43.011		34.21
704	CA			700	44.921	35.788	41.802		34.10
705	CB	LEU			46.407	35.560	42.179		32.00
706	CG			700	47.319	34.761	41.280		31.11
707		LEU			47.764	35.687	40.259		28.00
708		LEU			48.550	34.238	42.076		28.60
709	C			700	44.409	34.800	40.866		33.32 33.33
710 711	O N			700 701	44.504 43.814	35.041 33.697	39.691 41.348		34.11
712	CA	ASP			43.402	32.617	40.406		35.12
713	CB	ASP			42.894	31.383	41.064		33.80
714	CG	ASP			41.715	31.594	41.891		34.53
715	OD1	ASP			41.713	32.676	42.421		30.09
716		ASP			40.923	30.670	42.118		37.42
717	C	ASP			42.326	33.068	39.463		36.51
718	0	ASP			42.123	32.568			37.86
719	N			702	41.562	34.003	39.970		37.59

FIGURE 3N

A	В	С	D	E	F		G	Н		ľ	J
700	G.7.		_		40.65	_	24 520	20 11	^	1 00	26.66
720	CA	LYS			40.65		34.530	39.11			36.66
721	CB	LYS			39.34		34.752	39.97			39.28
722	CG	LYS			38.47		35.942	39.60		1.00	
723	CD	LYS			37.31		36.218	40.64		1.00	
724	CE	LYS			35.95		36.757	40.02			59.70
725	ΝZ	LYS			35.19		35.733	39.22			67.51
726	C	LYS			40.87		35.646	38.13			35.74
727	0	LYS			40.20		35.681	37.08			37.89
728	N			703	41.54		36.665	38.60			33.13
729	CA	PHE			42.20		37.643	37.76			36.62
730	CB			703	43.33		38.312	38.56			34.46
731	ÇG	PHE			44.01		39.505	37.87			38.02
732	CD1				43.17		40.498	37.33			25.27
733	CE1	PHE			43.73		41.626	36.75			33.70
734	CZ	PHE			45.13		41.763	36.64			34.23
735	CE2	PHE	Α	703	45.99		40.790	37.20			37.20
736	CD2	PHE		703	45.47		39.665	37.80			29.52
737	C	PHE	Α	703	42.87	6	36.911	36.59	9	1.00	35.72
738	0	PHE			42.62	9	37.269	35.55			37.70
739	N	LEU	Α	704	43.68	8	35.901	36.84		1.00	33.99
740	CA	LEU	Α	704	44.38	2	35.252	35.80	3	1.00	34.00
741	CB	LEU	A	704	45.21	3	34.181	36.37	3	1.00	32.88
742	CG	LEU	A	704	46.45	8	34.749	37.08	7	1.00	36.11
743	CD1	LEU	Α	704	47.35	2	33.579	37.37	4	1.00	37.94
744	CD2	LEU	Α	704	47.19	5	36.016	36.30	6	1.00	37.86
745	C	LEU	A	704	43.42	2	34.649	34.91	2	1.00	36.85
746	0	LEU	Α	704	43.71	5	34.499	33.72	1	1.00	35.55
747	N	ARG	Α	705	42.23	6	34.267	35.43	5	1.00	38.22
748	CA	ARG	Α	705	41.33	0	33.575	34.49	5	1.00	38.60
749	CB	ARG	Α	705	40.28	4	32.784	35.15	7	1.00	37.82
750	CG	ARG	Α	705	40.85	4	31.540	35.46	0	1.00	40.12
751	CD	ARG	Α	705	39.88	9	30.555	35.68	6	1.00	40.84
752	NE ·	ARG	Α	705	39.22	3	30.917	36.88	9	1.00	40.80
753	CZ	ARG	Α	705	39.62	1	30.530	38.09	4	1.00	48.75
754	NH1	ARG	Α	705	38.91	2	30.876	39.15	7	1.00	41.80
755	NH2	ARG	Α	705	40.70	0	29.778	38.23	9	1.00	48.73
756	C	ARG	Α	705	40.67	3	34.528	33.55	5	1.00	38.66
757	0	ARG	Α	705	40.32	0	34.170	32.47	3	1.00	40.65
758	N	GLU	Α	706	40.50	0	35.728	34.02	8	1.00	38.10
759	CA	GLU	Α	706	39.96	9	36.744	33.28	2	1.00	40.40
760	CB	GLU	Α	706	39.51	7	37.804	34.23	1	1.00	40.22
761	CG	GLU	Α	706	38.24	7	37.363	34.88	1	1.00	50.24
762	CD	GLU	Α	706	37.78	6	38.278	36.01	5	1.00	60.71
763	OE1	GLU	Α	706	36.71	1	37.952	36.57	8	1.00	61.83
764	OE2	GLU	Α	706	38.51	7	39.275	36.35	7	1.00	64.44
765	C	GLU			40.92		37.385	32.27	8	1.00	38.37
766	0	GLU			40.49		38.051	31.41	1	1.00	40.23
767	N	LYS			42.19		37.278	32.46			37.18
768	CA	LYS			43.14		38.027	31.60	2		35.98
769	CB	LYS			44.08		38.856	32.50			36.31
770	CG	LYS			43.43		40.070	33.15			31.25
771	CD	LYS			42.53		40.850	32.17			41.00

FIGURE 30

A	В	C	D	E		F	(G		H	I	J
770	CIT.	T 3/C	70	707		41.828	42.	150	2.7	801	1 00	43.91
772	CE			707 707		42.468	43.			199		46.63
773	NZ C			707		43.963	36.			907	1.00	
774				707	,	45.140	37.			851	1.00	
775 776	O N			708		43.310	35.			599		34.02
777	CA			708		43.961	34.			142		34.42
778	CB	ASP				42.937	33.			906		35.74
779	CG	ASP				43.549	32.			318		37.91
780		ASP				44.713	32.			373		46.66
781		ASP				42.940	31.			741		51.37
782	C	ASP				44.823	34.			843		33.85
783	0			708		44.332	35.			880	1.00	
784	N			709		46.076	34.			842	1.00	
785	CÁ			709		46.985	34.			796	1.00	
786	C			709		47.341	36.			734		33.50
787	0			709		48.010	36.			849		32.44
788	N			710		47.011	37.			715		33.77
789	CA			710		47.365	38.			521		35.02
790	СВ			710		46.198	39.			823	1.00	
791	CG			710		44.870	39.			228	1.00	
792	CD			710		43.843	40.			521	1.00	
793	OE1			710		44.173	41.			693	1.00	
794	OE2			710		42.704	39.			521	1.00	
795	C			710		48.602	39.			221		36.64
796	0			710		48.820	40.			192		34.62
797	N			711		49.403	38.			832		37.09
798	CA			711		50.510	38.			525		37.88
799	CB			711		50.414	38.			039	1.00	
800	CG			711		49.322	39.			812	1.00	38.60
801	CD1			711		48.302	38.			509	1.00	
802	CE1			711		47.359	39.		34.	196	1.00	36.81
803	CZ			711		47.377	40.		34.	129	1.00	43.70
804	CE2	PHE	Α	711		48.361	41.	361	33.	378	1.00	42.48
805	CD2	PHE				49.320	40.			722	1.00	36.32
806	C			711	!	51.731	38.	237	29.	795	1.00	38.37
807	0	PHE	A	711	!	51.653	37.	191	29.	189	1.00	38.38
808	N	SER	Α	712	!	52.829	38.	954	29.	832	1.00	37.51
809	CA	SER	Α	712	!	54.054	38.	463	29.	318	1.00	37.68
810	CB	SER	Α	712	!	55.019	39.	640	29.	207	1.00	33.41
811	OG	SER	Α	712	!	55.482	39.	865	30.	488	1.00	38.72
812	C	SER	Α	712	!	54.533	37.	373	30.	343	1.00	38.11
813	0	SER	Α	712	!	54.143	37.	370	31.	560	1.00	36.94
814	N	VAL	Α	713	!	55.345	36.4	430	29.	853	1.00	36.56
815	CA	VAL	A	713	9	55.970	35.	463	30.	743	1.00	38.74
816	CB	VAL	Α	713	!	56.860	34.	555	29.	902	1.00	40.25
817	CG1	VAL	Α	713	!	57.880	33.	741	30.	734	1.00	40.91
818	CG2	VAL			!	55.973	33.	661	29.	047	1.00	46.85
819	C	VAL	A	713	!	56.820	36.	172	31.	891	1.00	38.93
820	0	VAL	A	713	!	57.034	35.	653	33.	003	1.00	38.80
821	N	LEU	Α	714	!	57.279				621	1.00	38.01
822	CA	LEU	A	714	!	58.081	38.	031	32.	613	1.00	40.96
823	CB	LEU	A	714	!	58.951	39.	068	31.	898	1.00	40.30

FIGURE 3P

А	В	С	D	E	F	G	Н	I	J
824	CG	LEU	Α	714	60.120	39.781	32.561	1.00	45.88
825	CD1	LEU	Α	714	61.094	38.833	33.052	1.00	46.43
826	CD2	LEU	A	714	60.780	41.002	31.669	1.00	38.74
827	C	LEU	Α	714	57.168	38.638	33.698	1.00	40.29
828	0	LEU	Α	714	57.505	38.570	34.844	1.00	44.01
829	N	GLN	A	715	55.998	39.165	33.341	1.00	39.22
830	CA	GLN	Α	715	55.001	39.613	34.321	1.00	36.85
831	CB	GLN	Α	715	53.868	40.332	33.636	1.00	38.50
832	CG	GLN	Α	715	54.218	41.672	33.012	1.00	29.96
833	CD	GLN		715	53.075	42.067	32.167	1.00	28.87
834	OE1	GLN	Α	715	52.617	41.293	31.387	1.00	32.88
835	NE2	GLN		715	52.490	43.193	32.455	1.00	33.61
836	C	GLN		715	54.509	38.407	35.125	1.00	36.09
837	0	GLN		715	54.324	38.479	36.350	1.00	38.22
838	N	LEU		716	54.447	37.245	34.514	1.00	34.64
839	CA	LEU		716	54.000	36.106	35.305	1.00	34.14
840	CB	LEU		716	53.658	34.883	34.441	1.00	33.25
841	CG	LEU		716	52.373	35.072	33.597	1.00	34.69
842	CD1	LEU		716	52.021	33.922	32.684	1.00	40.42
843	CD2	LEU		716	51.151	35.391	34.465	1.00	35.13
844	C	LEU		716	55.008	35.742	36.325	1.00	36.34
845	0	LEU		716	54.687	35.526	37.487	1.00	38.96
846	N	VAL		717	56.247	35.640	35.901	1.00	35.71
847	CA	VAL		717	57.282	35.173	36.716	1.00	33.91
848	CB	VAL		717 717	58.571	35.031 34.711	35.931 36.866	1.00	35.17 29.77
849 850	CG1 CG2	VAL VAL		717	59.687 58.367	33.983	34.852	1.00	38.75
851	CG2	VAL		717	57.580	36.125	37.850	1.00	33.83
852	0	VAL		717	57.880	35.699	38.947	1.00	31.28
853	N	GLY		718	57.534	37.416	37.555	1.00	31.20
854	CA	GLY		718	57.503	38.426	38.592	1.00	35.27
855	C	GLY		718	56.292	38.282	39.565	1.00	36.66
856	0	GLY		718	56.491	38.537	40.791	1.00	39.82
857	N	MET		719	55.089	37.891	39.114	1.00	35.07
858	CA	MET		719	54.036	37.707	40.103	1.00	34.57
859	CB	MET		719	52.605	37.454	39.502	1.00	34.98
860	CG	MET	Α	719	52.011	38.624	38.740	1.00	38.87
861	SD	MET	A,	719	50.791	38.025	37.564	1.00	43.45
862	CE	MET	A	719	50.085	39.579	36.958	1.00	37.28
863	C	MET	Α	719	54.549	36.568	40.960	1.00	34.85
864	0	MET	Α	719	54.303	36.521	42.201	1.00	34.62
865	N	LEU	Α	720	55.287	35.643	40.362	1.00	33.93
866	CA	LEU	Α	720	55.655	34.523	41.175	1.00	35.01
867	CB	LEU	Α	720	56.042	33.265	40.370		34.91
868	CG	LEU			54.807	32.554	39.778		41.19
869	CD1	LEU	Α	720	55.348	31.681	38.652	1.00	33.86
870	CD2	LEU			54.125	31.703	40.866		35.22
871	C	LEU		720	56.796	34.940	42.127		34.33
872	0	LEU			56.915		43.175		33.94
873	N	ARG			57.633		41.741		35.51
874	CA	ARG			58.698	36.200	42.637		37.80
875	CB	ARG	A	721	59.987	36.862	42.044	1.00	38.19

FIGURE 3Q

A	В	С	D	E	F	G	;	Н	I	J
876	CG	ARG	Α	721	60.3	14 38.3	29 42	.432	1.00	43.45
877	CD	ARG			61.69	99 38.6	52 43	. 075	1.00	44.68
878	NE	ARG			61.6		68 43	. 738	1.00	46.01
879	CZ	ARG			62.1		23 45	.005		47.92
880	NH1	ARG			62.69			.760	1.00	42.62
881	NH2	ARG			62.0		26 45	.507	1.00	42.77
882	С	ARG			58.0		04 43	.840		35.74
883	0	ARG			58.3			.921	1.00	36.27
884	N	GLY			57.0			. 635	1.00	36.52
885	CA	GLY			56.39		22 44	.757	1.00	33.29
886	С	GLY			55.80			.691	1.00	32.31
887	0	GLY			56.1			.854	1.00	33.65
888	N			723	54.9	65 36.5	46 45	.211	1.00	30.16
889	CA	ILE	Α	723	54.5	43 35.5	18 46	.137	1.00	30.15
890	CB	ILE	Α	723	53.7	72 34.4	00 45	.387	1.00	29.03
891	CG1	ILE	Α	723	52.6	14 35.0	88 44	. 763	1.00	28.74
892	CD1	ILE	Α	723	51.89	90 34.3	11 43	. 667	1.00	22.43
893	CG2	ILE	Α	723	53.2	70 33.3	47 46	.367	1.00	23.88
894	C	ILE	Α	723	, 55.68	B2 34.9	39 46	. 875	1.00	29.85
895	0	ILE	Α	723	55.6	43 34.7	33 48	.086	1.00	28.93
896	N	ALA	Α	724	56.6	73 34.5	26 46	.105	1.00	30.46
897	CA	ALA	Α	724	57.7	62 33.7	58 46	.736	1.00	30.64
898	CB	ALA	Α	724	58.7	78 33.5	64 45	.694	1.00	32.41
899	C	ALA	Α	724	58.40	69 34.5	53 47	.912	1.00	29.69
900	0	ALA	Α	724	58.7	62 34.0	63 49	.021	1.00	26.55
901	N	ALA	Α	725	58.74	46 35.7	70 47	.606	1.00	27.76
902	CA	ALA	Α	725	59.3		50 48	.550		30.34
903	CB	ALA			59.33			.843		29.68
904	C	ALA			58.50			. 943	1.00	32.46
905	0	ALA			59.04			.069	1.00	32.65
906	N	GLY			57.1			.778	1.00	31.30
907	CA	GLY			56.2			. 888	1.00	
908	С			726	56.4			. 565	1.00	
909	0	GLY			56.5			.766	1.00	37.79
910	N	MET			56.5			. 825		33.96
911	CA			727	56.5			.482		36.78
912	CB	MET			56.3			.534	1.00	38.17
913	CG	MET			55.02			.128		35.85
914	SD	MET			53.7			.569		33.45
915	CE	MET			53.9			. 256		30.52 40.08
916	C	MET				04 33.1 32 32.4		.095 .994		40.52
917	O N	MET			58.13 59.0			.607		41.82
918	N Ca	LYS						. 222		43.04
919 920	CA CB	LYS LYS			60.30 61.5			.426		42.93
921	CG	LYS			62.8			374		45.08
922	CD	LYS			64.2			.788		48.13
923	CE	LYS			65.3			. 974		60.10
924	NZ	LYS			65.9			.965		59.07
925	C	LYS			60.2			629		43.72
926	0	LYS			60.7			703		42.16
927	N	TYR			59.50			.588		41.05
,			- •		33.3					

FIGURE 3R

Α	В	C	D	E		F	G	Н	I	J
928	CA	TYR	Δ	729	5	9.283	36.265	54.86	61 1 00	40.26
929	CB	TYR				8.511	37.417	54.5		36.34
930	CG			729		8.276	38.219	55.64		43.34
931	CD1	TYR				9.290	39.022	56.2		41.12
932	CE1	TYR				8.907	39.900	57.40		41.12
				729		7.600	39.837	57.80		41.14
933 934	CZ OH	TYR				6.977	40.579	58.88		40.30
	CE2	TYR				6.672	38.976	57.19		40.30
935	CD2	TYR				6.985	38.255	56.18		
936 937	CD2	TYR				8.534	35.355	55.86		42.10
		TYR				8.996	35.333	57.0		42.10
938	O N									42.02
939	N	LEU				7.379	34.814	55.42		39.74
940	CA	LEU				6.704	33.992	56.33		
941	CB	LEU				5.411	33.422	55.7		38.11
942	CG	LEU				4.356	34.521	55.42		
943	CD1	LEU				3.208	33.851	54.73		30.48
944	CD2	LEU		730		3.843	35.522	56.62		
945	C	LEU				7.615	32.961	56.80		40.93
946	0	LEU				7.590	32.614	58.09		44.06
947	N	ALA				8.379	32.366	56.00		41.66
948	CA	ALA				9.128	31.219	56.48		
949	СВ	ALA				9.665	30.304	55.30		42.98
950	C	ALA				0.252	31.695	57.42		43.66
951	0	ALA				0.645	31.018	58.30		44.04
952	N	ASN				0.709	32.885	57.2		44.35
953	CA	ASN				1.713	33.276	58.22		46.81
954	CB	ASN				2.560	34.350	57.60		43.35
955	CG	ASN				3.616	33.729	56.58		48.96
956	OD1	ASN				3.954	32.507	56.60		
957	ND2	ASN				4.077	34.565	55.6		51.65
958	C	ASN				1.050	33.532	59.64		47.03
959	0	ASN				1.593	33.105	60.64		47.94
960	N	MET				9.861	34.149	59.68		47.68
961	CA	MET				9.083	34.350	60.88		45.27
962	CB			733		7.872	35.218	60.69		43.96 48.30
963	CG	MET		733		8.018	36.674	60.28		
964	SD CE	MET		733		9.136 8.421	37.666 37.372	61.26		58.32 52.36
965		MET			_			62.74		
966	C	MET				8.590	33.013	61.34		45.93
967	0	MET				7.762	32.977	62.1		46.67
968	N	ASN				9.121	31.890	60.88		46.78
969	CA	ASN				8.546	30.632	61.34		47.20
970	CB	ASN				8.754	30.384	62.82		50.07
971	CG	ASN				0.243	30.038	63.14		56.81
972	OD1	ASN				0.886	30.656	64.04		57.16
973	ND2	ASN				0.803	29.077	62.3		
974	C	ASN				7.069	30.458	61.09		45.73
975	0	ASN				6.373	29.743	61.79		43.13
976	N	TYR				6.542	31.043	60.04) 44.71
977	CA	TYR				5.107	30.822	60.0		43.29
978	CB	TYR				4.443	32.126	59.92		42.22
979	CG	TYR	A	735	5.	3.029	32.009	59.72	24 1.00	41.13

FIGURE 3S

A	В	C	D	E	F	G	Н	I	J
980	CD1	TYR	А	735	52.152	32.131	60.814	1.00	40.42
981	CE1	TYR			50.811	32.085	60.664	1.00	47.06
982	CZ	TYR	Α	735	50.271	31.907	59.374	1.00	47.34
983	ОН	TYR			48.915	31.764	59.227	1.00	46.64
984	CE2	TYR			51.155	31.732	58.239	1.00	47.89
985	CD2	TYR			52.528	31.829	58.447		42.90
986	C	TYR			54.792	29.913	58.861		41.63
987	0	TYR			55.164	30.186	57.742		42.29
988	N	VAL			54.158	28.820	59.140		38.41
989	CA	VAL			53.937	27.923	58.084		39.18
990	СВ	VAL			53.963	26.643	58.559	1.00	
991		VAL			53.334	25.786	57.440	1.00	
992	CG2	VAL			55.465	26.273	59.020		41.99
993	C	VAL			52.508	28.121	57.602		40.83
994	0	VAL			51.554	27.827	58.342		37.18
995	N	HIS			52.358	28.570	56.348		38.45
996	CA	HIS			51.076	29.014	55.969	1.00	
997	CB	HIS			51.218	29.539	54.599		40.55
998	CG	HIS			50.007	30.193	54.135	1.00	
999		HIS			48.855	29.463			35.99
1000		HIS			47.910	30.315	53.492		39.74
1001	NE2	HIS			48.385	31.563	53.591		33.63
1002	CD2	HIS			49.695	31.497	54.039		31.88
1003	C	HIS			49.993	28.008	55.933		41.07
1004	0	HIS			48.797	28.237	56.357		44.04
1005	N	ARG			50.376	26.934	55.306		41.15
1006	CA	ARG			49.618	25.687	55.197		40.70
1007	CB	ARG			48.940	25.402	56.513	1.00	42.80
1008	CG	ARG			49.697	24.932	57.725	1.00	45.84
1009	CD	ARG			48.687	24.798	58.849	1.00	53.31
1010	NE	ARG			49.009	23.892	59.954	1.00	67.74
1011	CZ	ARG	A	738	48.085	23.420	60.827	1.00	72.67
1012	NH1	ARG			46.820	23.728	60.649	1.00	73.68
1013	NH2	ARG	Α	738	48.410	22.631	61.865	1.00	72.81
1014	С	ARG	Α	738	48.515	25.670	54.118	1.00	38.77
1015	0	ARG	Α	738	47.921	24.641	53.870	1.00	38.45
1016	N	ASP	Α	739	48.177	26.788	53.516	1.00	36.53
1017	CA	ASP	Α	739	47.072	26.753	52.631	1.00	36.55
1018	CB	ASP	Α	739	45.883	27.404	53.377	1.00	39.05
1019	CG	ASP	Α	739	44.538	27.308	52.614	1.00	42.96
1020	OD1	ASP	Α	739	43.754	28.312	52.665	1.00	43.61
1021	OD2	ASP	Α	739	44.148	26.255	52.038	1.00	39.35
1022	C	ASP	Α	739	47.535	27.617	51.504	1.00	36.75
1023	0	ASP	А	739	46.777	28.532	50.983	1.00	36.19
1024	N	LEU	Α	740	48.780	27.439	51.069	1.00	33.43
1025	CA	LEU	Α	740	49.061	28.504	50.134	1.00	33.57
1026	СВ	LEU	Α	740	50.481	28.864	50.075	1.00	33.24
1027	CG	LEU	А	740	50.940	29.335	48.750	1.00	31.68
1028	CD1	LEU	А	740	50.941	30.966	48.641	1.00	25.60
1029	CD2	LEU	A	740	52.323	28.912	48.706	1.00	23.37
1030	С	LEU	Α	740	48.490	28.150	48.796		33.56
1031	0	LEU	A	740	48.501	26.963	48.357	1.00	31.12

FIGURE 3T

A	В	С	D	E	F .	G	Н	I	J
1032	N	ALA	A	741	47.907	29.154	48.172	1.00	32.21
1033	CA			741	47.206	28.832	46.941	1.00	31.18
1034	CB			741	45.926	27.914	47.257		29.26
1035	С	ALA	Α	741	46.846	29.993	46.143	1.00	29.34
1036	0			741	46.668	31.011	46.680	1.00	33.20
1037	N	ALA	Α	742	46.670	29.881	44.843	1.00	30.74
1038	CA	ALA	Α	742	46.506	31.125	44.116	1.00	30.53
1039	CB	ALA	Α	742	46.415	30.932	42.505	1.00	29.25
1040	C	ALA	Α	742	45.285	31.834	44.608	1.00	29.77
1041	0	ALA	Α	742	45.243	33.003	44.528	1.00	31.53
1042	N	ARG	Α	743	44.245	31.119	44.944	1.00	30.98
1043	CA .	ARG	Α	743	43.077	31.884	45.424		34.86
1044	CB	ARG	Α	743	41.863	30.923	45.700		34.10
1045	CG			743	42.121	30.047	46.920		34.44
1046	CD			743	41.108	28.958	47.187		39.03
1047	NE			743	41.222	28.546	48.614		45.39
1048	CZ			743	41.915	27.457	49.044		48.15
1049		ARG			42.514	26.617	48.179		45.40
1050		ARG			42.006	27.199	50.343		47.01
1051	C			743	43.400	32.651	46.746		35.27
1052	0			743	42.567	33.390	47.192		35.06
1053	N			744	44.557	32.422	47.395		34.09
1054	CA			744	44.801	33.215	48.540		33.38
1055	CB			744 744	45.131 43.885	32.369 31.484	49.740 50.204		37.53 39.21
1056	CG	ASN			42.750	31.404	50.204		42.62
1057 1058		ASN			44.146	30.287	50.555		40.51
1058	C C			744	45.837	34.214	48.356		33.36
1060	0			744	46.457	34.589	49.341		35.07
1061	N			745	46.006	34.705	47.117	1.00	
1062	CA			745	46.897	35.733	46.854		28.67
1063	CB			745	47.832	35.223	45.714		30.71
1064	CG1			745	48.559	33.935	46.089		35.04
1065	CD1			745	49.267	33.990	47.383		35.54
1066	CG2			745	48.729	36.302	45.150		24.18
1067	C	ILE	Α	745	46.035	36.788	46.288	1.00	29.43
1068	0	ILE	Α	745	45.130	36.504	45.501	1.00	31.60
1069	N	LEU	Α	746	46.311	38.021	46.582	1.00	27.98
1070	CA	LEU	А	746	45.533	39.043	46.041	1.00	30.08
1071	CB	LEU	А	746	45.083	39.943	47.195	1.00	33.28
1072	CG	LEU	А	746	43.629	39.785	47.648	1.00	33.99
1073	CD1	LEU	Α	746	43.198	38.419	47.277	1.00	41.53
1074		LEU			43.681	39.973	49.163		38.93
1075	C	LEU			46.416	39.870	45.214		31.34
1076	0	LEU			47.672		45.411		33.08
1077	N	VAL			45.863		44.393		32.95
1078		VÀL			46.775				33.35
1079	CB	VAL				40.592			34.25
1080		VAL				41.171			32.32
1081		VAL				39.130			28.68
1082	C	VAL				42.728			35.15
1083	0	VAL	A	747	45.192	43.035	43.182	1.00	36.61

FIGURE 3U

A	В	С	D	E	F	G	Н	I	J
1084	N			748	47.265	43.612	43.005		38.24
1085	CA			748	46.877	45.028	42.924		38.34
1086	CB .			748	47.567	45.802	44.082		36.64
1087	CG			748	49.029	46.025	43.866		41.61
1088		ASN			49.862	46.322	44.892		43.62
1089		ASN			49.440	45.937	42.561		30.49
1090	C			748	47.108	45.643	41.577		39.45
1091	0			748	47.639	44.987	40.711		40.04
1092	N			749	46.695	46.895	41.373		42.73
1093	CA			749	46.786	47.496	40.099		46.89
1094	CB			749	46.385	48.978	40.082		48.87
1095	OG			749	45.668	49.315	41.225		54.36
1096	C			749	48.144	47.270	39.473		47.52
1097	0			749	48.120	47.006	38.275		50.51
1098	N			750	49.269	47.369	40.208		45.78
1099	CA			750	50.564	47.075	39.586		45.35
1100	CB			750	51.653	47.880	40.233		46.42
1101	CG			750	51.353	49.378	40.146	1.00	
1102		ASN			50.799	49.871	39.111	1.00	
1103		ASN			51.556	50.090	41.283		54.86
1104	C			750	50.867	45.596	39.508		45.29
1105	0			750	51.983	45.229	39.197		47.66
1106	N			751	49.900	44.715	39.759		43.51
1107	CA			751	50.329	43.316	39.610		41.03
1108	CB			751	50.906	43.089	38.217		38.31
1109	CG			751	50.061	43.748	37.120		41.64
1110		LEU			50.758	43.503	35.751		38.27
1111		LEU			48.627	43.252	36.999		28.14
1112	C			751	51.261	42.713	40.682	1.00	
1113	0			751	51.616	41.503	40.614		39.08
1114	N			752	51.532	43.481	41.722		38.48
1115	CA			752	52.201	42.927	42.911		37.62
1116	CB			752	52.407	44.027	43.985		41.07
1117	CG1	VAL			52.935	43.433	45.248		31.93
1118	CG2	VAL			53.374	45.187	43.434		39.70
1119	C	VAL			51.212	41.969	43.535	1.00	36.23
1120	0	VAL			50.109	42.327	43.656		37.11
1121	N	CYS			51.624	40.762	43.833		33.42
1122	CA	CYS			50.883	39.701	44.373		32.01
1123	CB	CYS		753	51.362	38.393	43.688		27.84
1124	SG	CYS			50.701	38.335	42.039		33.28
1125	C	CYS			51.225	39.605	45.855		32.33
1126	0	CYS			52.398	39.547	46.172		32.32
1127	N	LYS			50.219	39.528	46.741		32.94
1128	CA	LYS			50.507	39.386	48.166		32.10
1129	CB	LYS			50.162	40.696	48.875		33.13
1130	CG	LYS			50.605	41.963	48.135		29.06
1131	CD	LYS			50.285	43.144	49.026		35.71
1132	CE	LYS			50.643	44.415	48.261		35.80
1133	NZ	LYS			51.568	45.193	49.061		43.38
1134	C	LYS			49.841	38.219	48.816		32.31
1135	0	LYS	A	754	48.692	37.924	48.506	1.00	34.15

FIGURE 3V

A	В	C	D	E	F	G	Н	I	J
1136	N			755	50.518	37.575	49.758		31.55
1137	CA			755	49.978	36.428	50.386		33.31
1138	СВ			755	51.025	35.620	51.198		30.88
1139	CG1			755	50.350	34.441	51.795		32.21
1140	CG2			755	52.084	34.964	50.251		3424
1141	С			755	48.926	37.022	51.377		35.40
1142	0			755	49.168	38.016	52.005		32.54
1143	N			756	47.774	36.361	51.457		38.43
1144	CA			756	46.644	36.872	52.159		43.72
1145	CB			756	45.634	37.437	51.159		44.86
1146	OG			756	44.645	38.014	52.000		54.93
1147	С			756	46.074	35.651	52.814		43.72
1148	0	SER	Α	756	46.719	34.651	52.765		43.99
1149	N	ASP	Α	757	44.911	35.707	53.430		43.35
1150	CA			757	44.410	34.492	54.043		45.65
1151	CB			757	44.275	33.425	53.015		46.32
1152	CG	ASP	Α	757	43.724	32.150	53.635		52.75
1153	OD1	ASP	Α	757	44.124	30.984	53.230		56.00
1154	OD2	ASP	Α	757	42.867	32.274	54.510	1.00	43.97
1155	С	ASP	Α	757	45.196	33.850	55.204	1.00	46.33
1156	0	ASP	Α	757	45.641	32.720	55.119	1.00	45.10
1157	N	PHE	Α	758	45.277	34.549	56.314		47.63
1158	CA	PHE	Α	758	46.037	34.089	57.464	1.00	49.68
1159	CB	PHE	Α	758	46.847	35.258	58.006	1.00	44.29
1160	CG	PHE	Α	758	47.817	35.731	57.094	1.00	42.30
1161	CD1	PHE	Α	758	47.593	36.864	56.368	1.00	42.22
1162	CE1	PHE	A	758	48.598	37.322	55.442	1.00	39.71
1163	CZ	PHE	Α	758	49.746	36.532	55.255	1.00	36.81
1164	CE2			758	49.877	35.352	55.943	1.00	34.18
1165	CD2			758	48.975	34.983	56.849		40.00
1166	C			758	44.974	33.723	58.453		52.68
1167	0			758	44.200	34.528	58.838		57.15
1168	N			759	44.861	32.587	58.977		55.94
1169	CA			759	43.688	32.622	59.798		61.61
1170	C			759	43.267		60.339		65.29
1171	0			759	42.694	30.466	59.606		67.00
1172	N			760	43.669	31.122	61.603		68.87
1173	CA			760	43.342	30.071			70.34
1174	CB	ALA			42.221		63.474		72.37
1175	С			760	43.001		62.018		70.84
1176	0	ALA			43.734	27.741	62.273		72.10
1177	N	LYS			38.912	22.109	55.182		61.96
1178	CA			778	39.123	23.434	54.474		62.02
1179	CB	LYS			39.109	24.631	55.464		61.52
1180	CG			778	38.190	25.744	55.100		65.24
1181	CD	LYS			36.788	25.579	55.739		72.35
1182	CE			778	35.799	26.577	55.111		76.05
1183	NZ			778	34.359	26.088	55.161		78.40
1184	C	LYS			40.461	23.466	53.662		59.65
1185	0	LYS			40.624	24.295	52.798		60.18
1186	N			779		22.650			56.99
1187	CA	ILE	Α	779	42.634	22.716	53.087	1.00	54.46

FIGURE 3W

A	В	С	D	E	F	G		Н	I	J
1188	СВ	ILE	Α	779	44.00	3 22.7	69 53	.748	1.00	54.83
1189	CG1			779	44.10			.709		56.87
1190	CD1			779	45.31			.674	1.00	
1191	CG2			779	45.02			.634	1.00	
1192	C			779	42.60			.188	1.00	51.97
1193	0			779	42.66			.583		49.38
1194	N			780	42.59	5 21.7	96 50	.931		51.16
1195	CA	PRO	Α	780	42.50	9 20.7		.903	1.00	50.51
1196	CB	PRO	A	780	42.34	3 21.5	59 48	.651	1.00	51.35
1197	CG	PRO	A	780	43.26	0 22.6	89 48	.938	1.00	51.32
1198	CD	PRO	A	780	42.73	2 23.1	36 50	.382	1.00	49.94
1199	C	PRO	Α	780	43.74	9 19.9	36 49	.777	1.00	49.64
1200	0	PRO	Α	780	44.94	7 20.3	34 49	.770	1.00	49.57
1201	N	ILE	Α	781	43.45	9 18.6	72 49	.654		50.09
1202	CA	ILE	Α	781	44.55	9 17.7	37 49	.516	1.00	48.15
1203	CB	ILE	Α	781	43.97			.235		48.98
1204	CG1	ILE	Α	781	43.15	6 15.8	98 50	.458	1.00	49.76
1205	CD1	ILE	A	781	43.92	5 14.9	76 51	.333	1.00	45.76
1206	CG2	ILE		781	45.12			.961		49.83
1207	C	ILE	Α	781	45.51			.393		48.04
1208	0	ILE	Α	781	46.76	9 17.9		.510		48.83
1209	N	ARG			44.94			.261		47.13
1210	CA	ARG			45.80			.083		45.63
1211	CB	ARG			45.05			.769		47.26
1212	CG	ARG			44.02			.396		44.31
1213	CD	ARG		782	42.76			.519		46.69
1214	NE	ARG			42.14			.274		56.04
1215	CZ	ARG			41.46			.740		56.10
1216		ARG			40.97			.506		56.62
1217		ARG			41.30			.400	1.00	
1218	C	ARG			46.66			.954		44.90
1219	0	ARG			47.34			.928		43.83
1220	N	TRP TRP			46.61			.956		42.72
1221	CA CB	TRP		783 783	47.55			.995 .412		39.98 37.95
1222 1223	CG	TRP		783	46.86 46.47			.300		35.96
1223	CD1	TRP		783	47.14			.829		37.75
1225	NE1	TRP			46.44					33.74
1226		TRP			45.23			.689		27.42
1227		TRP			45.23			.630		27.27
1228		TRP			44.15			.665		39.26
1229		TRP			43.12			.774		36.66
1230		TRP			43.14			.847		39.76
1231		TRP			44.22			.792		24.85
1232	C	TRP			48.58			.036		38.70
1233	0	TRP			49.54			.357		35.32
1234	N	THR			48.40			.524		40.61
1235	CA	THR			49.17			.727		41.41
1236	СВ			784	48.22			.845		43.19
1237		THR			47.11			.014		45.29
1238				784	48.95			.200		34.46
1239	C			784	50.19			.543		42.11
	-		-	_			_ -			

FIGURE 3X

A	В	С	D	E	F	G	Н	I	J
1240	0	THR	Α	784	49.985	17.747	48.813	1.00	42.17
1241	N			785	51.327	18.906	50.196	1.00	42.96
1242	CA			785	52.418	17.963	50.141	1.00	44.73
1243	CB			785	53.572	18.448	50.832	1.00	42.17
1244	С			785	52.037	16.627	50.734	1.00	47.53
1245	0			785	51.473	16.538	51.822	1.00	46.77
1246	N	PRO	Α	786	52.460	15.590	50.029	1.00	48.19
1247	CA	PRO	Α	786	52.143	14.221	50.417	1.00	50.36
1248	CB	PRO	Α	786	53.099	13.338	49.569	1.00	50.74
1249	CG	PRO	Α	786	53.928	14.299	48.752	1.00	49.25
1250	CD	PRO	Α	786	53.440	15.726	48.965	1.00	46.85
1251	C	PRO	Α	786	52.522	14.054	51.936	1.00	52.21
1252	0	PRO	Α	786	51.679	13.490	52.651	1.00	51.09
1253	N	GLU	Α	787	53.714	14.492	52.403	1.00	53.11
1254	CA	GLU	Α	787	53.970	14.318	53.884	1.00	55.40
1255	CB	GLU	Α	787	55.401	14.738	54.382	1.00	54.09
1256	CG	GLU	Α	787	55.710	16.248	54.318		55.91
1257	CD	GLU		787	56.214	16.661	52.939		48.91
1258	OE1	GLU	Α	787	56.021	15.847	52.033		44.65
1259	OE2	GLU			56.840	17.727	52.812		45.31
1260	С	GLU	Α	787	52.848	15.012	54.726		55.92
1261	0			787	52.130	14.368	55.542		57.24
1262	N			788	52.713	16.318	54.544		54.35
1263	CA			788	51.644	16.988	55.186		54.04
1264	CB			788	51.446	18.323	54.578		53.00
1265	C			788	50.361	16.145	55.138		54.26
1266	0			788	49.670	16.086	56.112		54.80
1267	N			789	50.025	15.490	54.028		56.51
1268	CA			789	48.800	14.678	54.021		57.58
1269	CB			789	48.409	14.228	52.640		57.54
1270	CG1			789	47.712	15.332	51.828		59.40
1271	CD1			789	47.797	15.085	50.262		54.27
1272	CG2			789	47.309	13.160	52.772		60.10
1273	Ċ			789	48.914	13.392	54.862		58.22 57.15
1274	O N			789	48.062	13.049	55.692		
1275	N			790	49.990	12.659 11.382	54.690 55.316		59.69 61.39
1276	CA			790	49.932	10.325	54.444		61.41
1277	CB			790 790	50.549 51.936		54.315		61.74
1278 1279	OG C			790	50.226	11.364			63.87
1280	0			790	49.485	10.710	57.593		64.38
1281	N			791	51.144	12.202	57.303		63.52
1282	CA	TYR			51.439	12.287	58.665		66.15
1283	CB			791	52.945	12.283	58.781		68.10
1284	CG			791	53.565	11.076	58.118		72.28
1285	CD1	TYR			54.150	11.173	56.854		75.63
1286	CE1	TYR			54.755	10.071	56.241		78.33
1287	CZ			791	54.770	8.841	56.900		79.84
1288	OH			791	55.332	7.732	56.302		78.87
1289	CE2	TYR			54.210	8.722	58.176		79.39
1290		TYR				9.844			76.45
1291	C			791	50.974	13.612	59.238		66.97

FIGURE 3Y

A	В	С	D	E	F	G	Н	I	J
1292	0	TYR	A	791	51.182	13.912	60.434	1.00	66.84
1293	N	ARG	A	792	50.369	14.432	58.399		66.87
1294	CA	ARG		792	49.970	15:760	58.851	1.00	67.30
1295	CB	ARG	A	792	48.869	15.753	59.940	1.00	68.23
1296	CG	ARG	A	792	47.463	15.375	59.359	1.00	74.13
1297	CD	ARG	Α	792	46.869	14.030	59.780	1.00	82.23
1298	NE	ARG	Α	792	45.886	14.125	60.886	1.00	89.59
1299	CZ	ARG	Α	792	45.202	13.080	61.426	1.00	92.80
1300	NH1	ARG	Α	792	45.357	11.829	60.958	1.00	93.06
1301	NH2	ARG	Α	792	44.347	13.285	62.440	1.00	92.12
1302	C	ARG	A	792	51.197	16.520	59.320	1.00	65.45
1303	0	ARG	Α	792	51.139	17.269	60.315	1.00	65.77
1304	N	ALA	Α	793	52.306	16.318	58.611		63.00
1305	CA	ALA	A	793	53.519	17.103	58.883		61.10
1306	CB	ALA	A	793	54.867	16.228	58.776		60.85
1307	C	ALA	Α	793	53.648	18.397	58.049		59.08
1308	0			793	54.293	18.378	56.975		58.44
1309	N			794	53.105	19.517	58.578		56.19
1310	CA			794	53.275	20.777	57.901		52.79
1311	CB			794	52.133	21.718	58.149		51.44
1312	CG			794	50.889	21.224	57.553	1.00	
1313	CD1				50.266	20.110	58.096	1.00	
1314		PHE			49.177	19.633	57:537	1.00	
1315	CZ	,		794	48.642	20.230	56.394		57.08
1316	CE2			794	49.263	21.310	55.814		48.15
1317	.CD2	PHE			50.350	21.819	56.416	1.00	
1318	C			794	54.497	21.513	58.175		51.20
1319	0			794	54.691	21.921	59.279		51.64 49.90
1320	N CA			795	55.240	21.847 22.788	57.116 57.254		46.99
1321 1322	CA CB	THR		795	56.318 57.644	22.788	57.445	1.00	
1323	OG1				58.072	21.514	56.183		49.65
1323	CG2	THR			57.447	20.906	58.372		48.02
1325	C	THR			56.471	23.771	56.117		45.29
1326	0			795	55.655	23.860	55.164		43.69
1327	N			796	57.534	24.550	56.249		41.69
1328	CA			796	57.818	25.476	55.208		41.82
1329	CB	SER			58.981	26.331	55.547		39.66
1330	OG	SER			58.361	27.301	56.341		44.72
1331	C	SER			58.049	24.704	53.900		41.56
1332	0	SER			57.696	25.199		1.00	41.54
1333	N	ALA			58.524	23.473	53.999		40.13
1334	CA	ALA			58.846	22.725	52.848	1.00	42.53
1335	CB	ALA	Α	797	59.884	21.556	53.214	1.00	40.83
1336	C	ALA	Α	797	57.521	22.169	52.280	1.00	42.33
1337	0	ALA	Α	797	57.431	21.788	51.119	1.00	42.26
1338	N	SER	Α	798	56.545	22.072	53.157	1.00	40.76
1339	CA	SER	A	798	55.253	21.629	52.760	1.00	40.11
1340	CB	SER	A	798	54.431	21.573	54.027		41.27
1341	OG	SER	А	798	53.766	20.389	53.989		46.94
1342	C	SER	Α	798	54.772				39.12
1343	0	SER	Α	798	54.056	22.735	51.062	1.00	39.97

FIGURE 3Z

А	В	С	D	E	F	G	Н	I	J
1344	N	ASP	A	799	55.130	24.050	52.406	1.00	35.77
1345	CA			799	54.498	25.129	51.717		34.72
1346	CB			799	54.780	26.453	52.486		33.36
1347	CG			799	53.791	26.726	53.664	1.00	34.25
1348		ASP			52.668	26.165	53.890	1.00	36.89
1349		ASP			54.068	27.559	54.447		37.78
1350	С			799	55.132	25.237	50.316	1.00	35.69
1351	0			799	54.570	25.868	49.348	1.00	37.88
1352	N	VAL	Α	800	56.387	24.819	50.252	1.00	34.31
1353	CA	VAL	Α	800	57.112	24.959	49.039	1.00	34.33
1354	CB	VAL	Α	800	58.663	24.654	49.163	1.00	34.63
1355	CG1	VAL	Α	800	59.248	24.426	47.761	1.00	30.86
1356	CG2	VAL	А	800	59.460	25.863	49.911	1.00	29.88
1357	C	VAL	А	800	56.427	24.040	48.023	1.00	34.69
1358	0	VAL	Α	800	56.251	24.480	46.945	1.00	36.80
1359	N	TRP	Α	801	56.055	22.823	48.359	1.00	32.29
1360	CA	TRP	А	801	55.170	22.045	47.475		34.84
1361	CB	ŤRΡ	А	801	54.679	20.731	48.117		35.44
1362	CG	TRP	A	801	53.843	19.907	47.285	1.00	33.44
1363	CD1	TRP	А	801	52.561	20.102	46.984		32.49
1364	NE1	TRP	А	801	52.070	19.046	46.260		32.97
1365	CE2				53.073	18.136	46.097	1.00	
1366	CD2	TRP			54.183	18.623	46.756	1.00	
1367	CE3	TRP			55.320	17.800	46.841		38.46
1368	CZ3	TRP			55.378	16.614	46.143		33.13
1369	CH2	TRP			54.264	16.152	45.448		37.50
1370	CZ2	TRP			53.088	16.888	45.430		42.25
1371	C			801	53.951	22.760	47.036		34.91
1372	0			801	53.531	22.621	45.934		38.09
1373	N			802	53.355	23.576	47.890		35.76
1374	CA			802	52.126	24.274	47.503		31.87
1375	CB			802	51.515	24.963	48.746		33.54
1376	OG			802	50.899	23.899	49.521		30.64
1377	C			802	52.429	25.304	46.557		31.93
1378	O N			802	51.690	25.509 26.007	45.608	1.00	34.62 30.27
1379 1380	N			803 803	53.536 - 53.933	27.101	46.779 45.905	1.00	
1380	CA	PHE			55.219				
1382	CG	PHE			55.817		45.639		32.84
1382		PHE			56.825				30.14
1384		PHE			57.313	29.296			28.45
1385	CZ			803	56.814				26.76
1386		PHE			55.846				30.61
1387		PHE			55.372	29.962	45.745		26.06
1388	C			803	54.263	26.610	44.484		30.18
1389	0	PHE			54.033	27.263	43.432		27.18
1390	N	GLY			54.777	25.406	44.421		32.24
1391	CA	GLY			54.953	24.865	43.033		33.84
1392	C	GLY			53.552	24.724	42.358		33.65
1393	o	GLY			53.373				31.75
1394	N			805	52.558				33.22
1395	CA			805	51.181				33.26

FIGURE 3AA

A	В	С	D	E		F		G	H	I	J
1396	CB	ILE	Α	805	50.	229		.528	43.503		33.65
1397	CG1			805		811		.097	43.852		37.12
1398	CD1			805		975		032	42.698		32.87
1399	CG2			805		823		.678	43.010		32.49
1400	С			805		696		.579	42.206		31.48
1401	0			805		103		.710	41.183		35.71
1402	N			806		019		.638	42.935		28.75
1403	CA			806		549		.991	42.575		25.41
1404	CB			806		961		.014	43.621		25.04
1405	CG1	VAL				941		.522	43.191		21.16
1406	CG2	VAL				157		.790	45.007		23.21
1407	C			806		341		.242	41.357		29.80
1408	0			806		912		.993	40.455		29.17
1409	N			807		538		.649	41.280		30.71
1410	CA			807		344		.966	40.092		31.44
1411	CB			807		785		.399	40.149		32.92
1412	CG			807		817		.157	41.066		31.62
1413	SD			807	-	439		.395	40.955		39.41
1414	CE			807		070		.142	40.672		45.05
1415	С			807		606		.493	38.830		31.38
1416	0			807		491		.212	37.876		33.09
1417	N			808		936		.352	38.875		31.98
1418	CA			808		347		.777	37.672		32.34
1419	CB			808		102		.315	38.067		33.08
1420	CG			808		501		.517	37.005		36.11
1421	CD1			808		163		.792	36.077		36.58
1422	NE1			808		257		.139	35.281		38.43
1423	CE2			808		005		.468	35.660		33.35
1424	CD2			808		123		.335	36.754		31.70
1425	CE3			808		968		.831	37.345		35.04
1426	CZ3			808		744		.452	36.868		36.54
1427	CH2			808		638		.571	35.743		38.94
1428	CZ2	TRP				760		.047	35.138		38.69
1429	C			808		064		.516	37.482		33.39
1430	0			808		612		.851	36.402		34.70
1431	N			809		457		.832	38.629		33.47
1432	CA			809		354		.714	38.567		30.38
1433	CB	GLU				563		.010	39.941		30.54
1434	CG	GLU				069		.930	40.924		28.60
1435	CD	GLU				429		.611	42.127		33.46
1436		GLU				269		.166	42.033		31.67
1437		GLU				163		.747	43.156		40.29
1438	C	GLU				610		.024	37.793		29.74
1439	0	GLU				798		.552	36.933		30.79
1440	N	VAL				656		.723	38.167		28.13
1441	CA	VAL		•		889		.000	37.520		26.64
1442	CB	VAL				022		.716	38.242		26.67
1443		VAL				575		.853	37.310		22.89
1444	CG2	VAL				493		.103	39.725		27.59
1445	C	VAL				319		.755	35.999		28.59
1446	0	VAL				854		.404	35.114		24.03
1447	N	MET	Α	811	ъl.	055	29	.682	35.705	1.00	30.08

FIGURE 3AB

A	В	С	D	E	F	G	Н	I	J
1448	CA	MET	Α	811	51.499	29.612	34.339	1.00	31.44
1449	СВ	MET			52.744	28.783	34.201	1.00	35.04
1450	CG	MET			54.001	29.305	35.125	1.00	31.45
1451	SD	MET			54.298	30.999	34.729	1.00	37.47
1452	CE	MET	Α	811	54.782	30.847	33.012	1.00	32.94
1453	С	MET			50.347	29.060	33.524	1.00	34.61
1454	0	MET	A	811	50.403	29.178	32.332	1.00	32.60
1455	N	THR	А	812	49.276	28.501	34.133	1.00	34.24
1456	CA	THR	Α	812	48.198	28.074	33.241	1.00	32.52
1457	CB	THR	Α	812	47.466	26.795	33.649	1.00	34.00
1458	OG1	THR	Α	812	47.141	26.876	35.053	1.00	32.67
1459	CG2	THR	Α	812	48.398	25.639	33.662	1.00	30.33
1460	C	THR	Α	812	47.135	29.096	33.341	1.00	31.91
1461	0	THR	А	812	46.025	28.855	32.943	1.00	30.76
1462	N	TYR	А	813	47.464	30.243	33.834	1.00	31.56
1463	CA	TYR	А	813	46.387	31.261	33.929	1.00	31.70
1464	CB	TYR	Α	813	46.014	31.896	32.589	1.00	29.74
1465	CG	TYR			47.044	32.836	31.958		30.09
1466	CD1	TYR			48.104	32.376	31.114		28.85
1467	CE1	TYR	A	813	49.010	33.279	30.612		29.29
1468	CZ	TYR	Α	813	48.842	34.593	30.910		29.69
1469	OH	TYR			49.541	35.655	30.375		38.24
1470	CE2	TYR			47.824	35.015	31.708		31.05
1471	CD2	TYR			46.969	34.162	32.203		29.25
1472	C	TYR			45.134	30.738	34.656		30.85
1473	Ο.	TYR			44.083	30.936	34.220		30.55
1474	N	GLY			45.270	30.031	35.753		33.19
1475	CA	GLY			44.090	29.747	36.568		35.27
1476	C	GLY			43.411	28.377	36.403		37.11
1477	0	GLY			42.283	28.190	36.933		33.77
1478	N	GLU			44.027	27.436	35.672		36.20
1479	CA	GLU			43.465	26.106	35.683		39.73
1480	CB	GLU			44.122	25.206	34.568		39.41
1481	CG	GLU			43.383	23.879	34.352		45.14
1482	CD	GLU GLU			41.799	24.015	34.235		55.70 48.24
1483	OE1	GLU			41.019 41.307	24.346 23.789	35.224 33.053		64.63
1484	OE2 C	GLU			43.505	25.458	37.133		40.38
1485 1486		GLU			44.323				41.33
1487	N O	ARG			42.636				41.29
1488	CA	ARG			42.531				42.57
1489	CB	ARG			41.035		38.997		43.10
1490	CG	ARG			40.769	21.927	39.483		46.76
1491	CD	ARG			39.291	21.462	39.802		54.39
1492	NE	ARG			39.376	20.573	40.974		59.04
1493	CZ	ARG			39.408	21.041	42.240		63.78
1494		ARG			39.513	20.179	43.233		65.53
1495		ARG			39.304	22.384	42.511		59.05
1496	C	ARG			43.464		38.721		41.97
1497	0	ARG			43.398				42.38
1498	N	PRO			44.469				43.68
1499	CA	PRO			45.379				41.81
	1								

FIGURE 3AC

A	В	С	D	E	F	G	Н	I	J
1500	СВ	PRO	Α	817	46.156	21.699	40.929	1.00	41.78
1501	CG	PRO	Α	817	46.031	23.202	41.122	1.00	43.11
1502	CD	PRO	Α	817	44.749	23.678	40.560	1.00	40.66
1503	С	PRO	Α	817	44.627	20.101	39.695	1.00	44.30
1504	0	PRO	Α	817	43.467	19.877	40.271	1.00	45.86
1505	N	TYR	Α	818	45.189	19.255	38.843	1.00	44.92
1506	CA	$\mathbf{T}\mathbf{Y}\mathbf{R}$	Α	818	44.739	17.910	38.593	1,.00	45.34
1507	CB	TYR	Α	818	44.740	17.159	39.884	1.00	43.91
1508	CG	TYR	Α	818	46.093	17.345	40.535		42.86
1509	CD1	\mathbf{T} YR			47.185	16.479	40.253		38.28
1510	CE1	TYR			48.459	16.660	40.852		37.76
1511	CZ			818	48.610	17.633	41.743	1.00	
1512	OH			818	49.875	17.735	42.212		42.19
1513	CE2	TYR			47.577	18.531	42.049		33.24
1514	CD2	TYR			46.316	18.406	41.423		37.98
1515	C			818	43.336	17.995	38.033		47.01
1516	0			818	42.518	17.049	38.110		48.49
1517	N			819	43.005	19.164	37.505		47.05
1518	CA			819	41.701	19.253	36.867		50.46
1519	CB			819	41.740	18.432	35.528		48.43
1520	CG CD1			819	42.829	18.844	34.728 34.004		46.58 49.18
1521	CD1 NE1	TRP TRP			42.959 44.228	20.031	33.441		43.18
1522 1523	CE2	TRP			44.918	18.980	33.793		43.12
1524	CD2	TRP			44.087	18.187	34.609		47.93
1525	CE3			819	44.579	16.961	35.056		49.44
1526	CZ3	TRP			45.822	16.613	34.720		46.77
1527	CH2	TRP			46.585	17.392	33.912		42.84
1528	CZ2	TRP			46.157	18.598	33.464		45.34
1529	C			819	40.560	18.743	37.751		50.78
1530	0			819	40.418	19.134	38.920	1.00	
1531	N			820	39.757	17.855	37.170	1.00	53.15
1532	CA	GLU	Α	820	38.614	17.241	37.872	1.00	54.37
1533	CB	GLU	Α	820	37.449	16.941	36.924	1.00	54.32
1534	CG	GLU	Α	820	36.366	18.002	36.896	1.00	57.57
1535	CD			820	36.972	19.390	36.838	1.00	61.97
1536		GLU			36.651	20.232	37.703		63.58
1537	OE2	GLU	Α	820	37.815	19.635			65.58
1538	C	GLU			38.939				54.50
1539	0			820	38.032				56.40
1540	N	LEU			40.212				55.83
1541	CA	LEU			40.604	14.432	39.369		54.87
1542	CB	LEU			42.050	14.101	39.090		54.66
1543	CG	LEU			42.599	13.702	37.713		55.17
1544		LEU			44.138	14.023	37.650		59.74
1545		LEU			42.372	12.223	37.358		57.81
1546	C	LEU			40.311	14.322	40.862		55.57
1547	O N	LEU SER			40.184 40.208	15.328	41.610		52.91 55.96
1548	N CA			822	39.800	13.053 12.777	41.283 42.619		56.75
1549 1550	CB			822	39.132		42.709		57.57
1551	OG			822	40.163	10.441			61.05
1001	J	CER	Λ	044	20.103	10.111	12./27	1.00	31.03

FIGURE 3AD

A	В	С	D	Е	F	G	Н	I	J
1552	Ċ	SER	Α	822	41.015	12.742	43.471	1.00	56.82
1553	Ō			822	42.111	12.351	43.029		55.43
1554	N			823	40.752	13.039	44.733		57.38
1555	CA			823	41.802	13.209	45.699		58.87
1556	CB	ASN	Α	823	41.242	13.615	47.073	1.00	
1557	CG			823	40.815	15.094	47.094	1.00	60.32
1558	OD1	ASN	Α	823	41.592	15.963	46.785		63.73
1559	ND2	ASN			39.582	15.363	47.432		61.31
1560	C			823	42.513	11.941	45.660	1.00	59.12
1561	0	ASN	Α	823	43.753	11.872	45.759	1.00	60.64
1562	N	HIS	Α	824	41.733	10.936	45.381	1.00	58.77
1563	CA	HIS	Α	824	42.274	9.608	45.413	1.00	60.00
1564	CB	HIS	A	824	41.115	8.627	45.445	1.00	60.99
1565	CG	HIS	Α	824	41.565	7.246	45.256	1.00	67.03
1566	ND1	HIS	Α	824	42.251	6.566	46.238	1.00	72.16
1567	CE1	HIS	Α	824	42.594	5.370	45.772	1.00	77.00
1568	NE2	HIS	Α	824	42.189	5.271	44.513	1.00	75.73
1569	CD2	HIS	Α	824	41.551	6.441	44.161	1.00	74.03
1570	С	HIS	Α	824	43.240	9.346	44.223	1.00	58.19
1571	0	HIS	Α	824	44.439	9.014	44.396	1.00	55.80
1572	N	GLU	Α	825	42.701	9.531	43.014	1.00	57.37
1573	CA	GLU	Α	825	43.514	9.516	41.785	1.00	56.22
1574	CB	GLU	Α	825	42.623	10.008	40.632	1.00	57.84
1575	CG	GLU	Α	825	41.881	8.907	39.881	1.00	62.50
1576	CD	GLU	Α	825	40.412	9.114	39.860	1.00	67.90
1577	OE1	GLU	A	825	39.948	10.076	39.213	1.00	70.44
1578		GLU	A	825	39.725	8.297	40.518		74.63
1579	C	GLU	Α	825	44.764	10.399	42.063		54.94
1580	0			825	45.937	9.927	42.067		54.45
1581	N			826	44.529	11.648	42.467	1.00	
1582	CA			826	45.667	12.540	42.776		52.93
1583	CB			826	45.208	13.870	43.319		51.81
1584		VAL			46.447	14.871	43.452		52.68
1585	CG2	VAL			44.197	14.432	42.370		51.90
1586	C			826	46.759	11.943	43.687		53.42
1587	0			826	47.967	11.917	43.378		53.40
1588	N			827	46.363	11.447	44.821		53.41
1589	CA			827	47.422	10.969			55.16
1590	CB	MET			47.018	10.882	47.148		55.87
1591	CG			827	45.490	10.429	47.445		60.83
1592	SD			827	44.615	10.847			65.49
1593	CE			827	46.288	11.405	49.883		54.71
1594	C	MET			48.133	9.757	44.935		54.89
1595	O N	MET			49.401	9.704	44.875		55.10
1596	N	ALA			47.375	8.861	44.295		55.10
1597	CA	ALA			48.085	7.757	43.600		55.33
1598	CB	ALA			47.165	6.654	43.057		54.77
1599 1600	C 0	ALA ALA			49.049	8.267 7. 7 92	42.521 42.403		54.77 54.26
	N	ALA			50.167	9.315	42.403		55.62
1601	CA	ALA			48.698 49.672	9.315	40.804		56.05
1602 1603	CB	ALA			49.103	10.831	39.898		56.37
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FIGURE 3AE

A	В	С	D	E	F	G	H	I	J
	_								
1604	C			829	50.966	10.177	41.468		56.31
1605	0			829	52.116	9.756	41.108	1.00	
1606	N			830	50.765	11.020	42.471	1.00	
1607	CA			830	51.891	11.651	43.112	1.00	
1608	CB			830	51.446	12.581	44.293		57.35
1609	CG1			830	50.835	13.861	43.719		56.71
1610	CD1			830	51.574	14.320	42.496		47.37
1611	CG2	ILE			52.641	12.975	45.149		52.92
1612	C			830	52.767	10.611	43.637		58.16
1613	0			830	54.003	10.637	43.431		58.31
1614	N			831	52.120	9.692	44.344	1.00	
1615	CA			831	52.883	8.672	45.016		60.79
1616	CB	ASN			52.033	7.966	46.046		62.19
1617	CG			831	51.972	8.768	47.324		65.87
1618		ASN			52.993	9.400	47.727		66.49
1619		ASN			50.781	8.826	47.934		68.01
1620	C	ASN			53.492	7.757	44.044		59.66
1621	0	ASN			54.558	7.248	44.274		58.77
1622	N	ASP			52.860	7.609	42.896	1.00	
1623	CA	ASP			53.530	6.790	41.905		60.01
1624	CB	ASP			52.494	6.118	41.014		60.55
1625	CG	ASP			52.076	4.698	41.576		66.55
1626		ASP			51.135	4.051	41.007		71.66
1627		ASP			52.672	4.151	42.569		63.91
1628	C	ASP			54.697	7.455	41.121		59.37
1629	0	ASP			55.088	6.979	40.039		58.56
1630	N	GLY			55.293	8.525	41.664		58.64
1631	CA	GLY			56.220	9.303	40.850		57.55
1632	C	GLY			55.529	9.892	39.615	1.00	
1633	0	GLY			55.730	9.408	38.503		61.73
1634	N	PHE			54.711	10.932	39.806		55.50
1635	CA	PHE			53.992	11.588	38.713		52.71
1636	CB	PHE			52.692	10.831	38.438		52.86
1637	CG	PHE			52.758	9.760	37.377		55.68
1638	CD1	PHE			53.292	9.991	36.064		61.07
1639	CE1	PHE			53.276	8.953	35.053	1.00	
1640	CZ	PHE			52.739	7.624	35.386		60.52
1641	CE2				52.202	7.400	36.702	1.00	56.50
1642		PHE			52.210	8.481	37.656		60.30
1643	C	PHE			53.471	12.969	39.156		50.70
1644	0	PHE			52.879	13.061	40.234		50.00
1645	N	ARG			53.578	13.973	38.269		47.79
1646	CA	ARG			53.278	15.397	38.529		47.62
1647	CB	ARG			54.544	16.240	38.538		47.50
1648	CG	ARG			55.739	15.796	39.492		48.70
1649	CD	ARG			55.161	15.694	40.870		48.58
1650	NE	ARG			56.010	15.092	41.866		46.46
1651	CZ	ARG			55.778	13.923	42.395		45.45
1652	NH1				54.763	13.179	41.994		49.16
1653		ARG			56.575	13.478	43.301		47.75
1654	C	ARG			52.392	16.027			44.98
1655	0	ARG	A	835	52.160	15.415	36.403	1.00	46.68

FIGURE 3AF

A	В	С	D	E	F	G	Н	I	J
1656	N	LEU	Α	836	51.883	17.246	37.678	1.00	42.81
1657	CA			836	51.065	17.947	36.699		41.01
1658	СВ	LEU	Α	836	50.651	19.385	37.117	1.00	38.39
1659	CG			836	49.702	19.386	38.291	1.00	40.70
1660	CD1	LEU	Α	836	49.697	20.808	38.794	1.00	38.83
1661	CD2	LEU	Α	836	48.341	18.855	37.832	1.00	33.85
1662	C			836	51.944	18.162	35.569	1.00	38.14
1663	0	LEU	Α	836	53.047	18.472	35.801	1.00	38.29
1664	N	PRO	Α	837	51.413	18.144	34.359	1.00	38.07
1665	CA	PRO	Α	837	52.214	18.316	33.157	1.00	36.29
1666	CB	PRO	Α	837	51.232	17.819	32.075	1.00	36.93
1667	CG	PRO	Α	837	49.907	18.505	32.492	1.00	35.54
1668	CD	PRO	Α	837	49.973	18.141	34.008	1.00	37.87
1669	C	PRO	Α	837	52.525	19.778	32.964	1.00	36.09
1670	0	PRO	Α	837	51.936	20.719	33.673	1.00	34.39
1671	N	THR	Α	838	53.406	20.032	32.013	1.00	34.01
1672	CA	THR	Α	838	53.894	21.359	31.903	1.00	35.98
1673	CB	THR	Α	838	55.120	21.485	30.963	1.00	36.64
1674	OG1	THR	Α	838	55.395	22.892	30.765	1.00	39.83
1675	CG2	THR	Α	838	54.736	21.181	29.545	1.00	38.71
1676	C	THR	Α	838	52.803	22.116	31.252	1.00	38.36
1677	0	THR	Α	838	52.197	21.670	30.274	1.00	39.45
1678	N	PRO	Α	839	52.619	23.313	31.726	1.00	36.96
1679	CA	PRO	A	839	51.719	24.197	31.114^{-}		37.46
1680	CB	PRO	Α	839	51.724	25.405	32.037		34.44
1681	CG	PRO	Α	839	52.681	25.139	33.091		33.53
1682	CD			839	53.318	23.890	32.865		37.82
1683	С			839	52.285	24.602	29.749		38.53
1684	0	PRO	Α	839	53.481	24.718	29.536		40.65
1685	N			840	51.382	24.872	28.840		40.11
1686	CA			840	51.632	25.423	27.501		40.90
1687	CB			840	50.230	25.730	26.953		42.06
1688	CG	MET			50.129	26.167	25.481		50.27
1689	SD	MET			50.014	24.569	24.486		67.03
1690	CE	MET			51.027	25.324	23.049		53.52
1691	C			840	52.554	26.728	27.544		40.78
1692	0	MET			52.331	27.704	28.311		41.90
1693	N ·				53.600	26.738			39.46
1694	CA	ASP			54.541	27.802	26.665		38.39
1695	CB	ASP			53.847	28.967	26.104		36.97
1696	CG	ASP			53.255	28.676	24.629		40.53
1697		ASP			53.550	27.617	23.972		39.77
1698		ASP			52.445	29.466	24.066		36.62
1699	C	ASP			55.291	28.055	28.007		39.55
1700	0	ASP			55.749	29.129	28.326		41.50
1701	N	CYS			55.381	27.056	28.840		39.14
1702	CA	CYS			56.121	27.250	30.088		37.64
1703	CB	CYS			55.781	26.076	31.018		35.73
1704	SG	CYS			56.126	26.564	32.674		37.11
1705	C	CYS			57.616	27.200	29.840		36.94
1706	0	CYS			58.077		29.219		33.74
1707	N	PRO	A	843	58.352	28.267	30.217	1.00	37.65

FIGURE 3AG

A	В	С	D	E	F	G	Н	I	J
1708	CA	PRO	Α	843	59.804	28.178	30.251	1.00	34.75
1709	CB			843	60.257	29.383	31.062	1.00	31.74
1710	CG			843	59.216	30.413	30.790	1.00	38.14
1711	CD			843	57.864	29.626	30.588	1.00	36.86
1712	C			843	60.258	26.981	30.973	1.00	34.58
1713	Ō			843	59.616	26.646	32.033		34.71
1714	N			844	61.364	26.414	30.439	1.00	30.44
1715	CA			844	61.947	25.239	30.957	1.00	32.01
1716	CB			844	63.155	24.861	30.092	1.00	32.60
1717	OG			844	63.939	23.905	30.735	1.00	32.71
1718	C			844	62.421	25.519	32.326	1.00	
1719	Ö			844	62.327	24.669	33.152	1.00	34.58
1720	N	ALA			62.988	26.690	32.593		34.49
1721	CA			845	63.384	26.961	34.006		36.49
1722	CB			845	64.315	28.212	34.109		35.62
1723	C	ALA			62.124	27.066	34.982		34.14
1724	Ö			845	62.137	26.522	36.021		35.47
1725	N			846	60.992	27.590	34.558	1.00	
1726	CA			846	59.787	27.597	35.457	1.00	
1727	CB			846	58.778	28.539	34.866	1.00	33.95
1728	CG1			846	59.535	29.848	34.737	1.00	
1729	CD1			846	59.817	30.375	36.417		26.15
1730	CG2			846	57.462	28.631	35.735		28.18
1731	C.			846	59.233	26.236	35.656	1.00	32.51
1732	Ō			846	59.054	25.847	36.786	1.00	31.68
1733	N			847	59.145	25.413	34.603	1.00	35.30
1734	CA			847	58.714	23.984	34.822	1.00	
1735	СВ			847	58.713	23.167	33.520	1.00	35.69
1736	CG			847	57.927	21.911	33.661	1.00	32.14
1737	CD1			847	58.477	20.696	33.310	1.00	27.77
1738	CE1	TYR	Α	847	57.759	19.516	33.469	1.00	33.54
1739	CZ			847	56.522	19.509	34.064	1.00	31.43
1740	OH	TYR	Α	847	55.943	18.320	34.231	1.00	40.26
1741	CE2	TYR	Α	847	55.917	20.681	34.490	1.00	35.09
1742	CD2	TYR	Α	847	56.645	21.928	34.253	1.00	32.81
1743	C	TYR	Α	847	59.577	23.180	35.723	1.00	36.62
1744	0	TYR	Α	847	59.090	22.401	36.510		38.41
1745	N	GLN	Α	848	60.874	23.301	35.605	1.00	38.13
1746	CA	GLN	Α	848	61.806	22.493	36.466	1.00	39.42
1747	СВ	GLN	Α	848	63.262	22.533	35.863	1.00	42.35
1748	CG	${\tt GLN}$	Α	848	63.313	21.927	34.477	1.00	38.83
1749	CD	GLN	Α	848	62.999	20.404	34.549	1.00	44.22
1750	OE1	GLN	Α	848	62.228	19.877	33.736	1.00	48.28
1751	NE2	GLN	Α	848	63.569	19.735	35.485	1.00	33.20
1752	C	${\tt GLN}$	Α	848	61.821	22.902	37.950	1.00	36.31
1753	0	GLN	A	848	61.762	22.045	38.829		35.55
1754	N	LEU	A	849	61.847	24.194	38.200	1.00	37.37
1755	CA	LEU	Α	849	61.716	24.680	39.552	1.00	38.40
1756	CB	LEU	A	849	61.552	26.151	39.507	1.00	37.22
1757	CG	LEU	Α	849	61.237	26.406	40.933	1.00	36.60
1758	CD1	LEU	Α	849	62.551	26.128	41.744	1.00	24.80
1759	CD2	LEU	A	849	60.902	27.913	40.922	1.00	33.30

FIGURE 3AH

A	В	С	D	E	F	G	Н	I	J
1760	С	LEU	Α	849	60.521	24.099	40.250	1.00	39.79
1761	0			849	60.540	23.685	41.468		43.91
1762	N	MET	Α	850	59.445	24.005	39.489		39.24
1763	CA			850	58.240	23.461	40.122		39.96
1764	CB	MET	А	850	56.904	23.372	39.299	1.00	40.95
1765	CG	MET	Α	850	56.413	24.449	38.405	1.00	41.55
1766	SD			850	55.117	23.680	37.431	1.00	39.78
1767	CE	MET	Α	850	54.574	24.992	36.847	1.00	18.82
1768	C	MET	Α	850	58.422	22.040	40.423	1.00	37.52
1769	0	MET	Α	850	57.783	21.573	41.370	1.00	38.53
1770	N	MET	Α	851	58.853	21.295	39.415	1.00	35.10
1771	CA	MET	Α	851	59.106	19.877	39.608	1.00	37.40
1772	CB	MET	Α	851	59.826	19.275	38.407	1.00	36.06
1773	CG	MET	Α	851	58.932	19.130	37.200	1.00	35.21
1774	SD	MET	Α	851	57.537	18.184	37.411	1.00	43.74
1775	CE	MET	Α	851	58.198	16.716	37.455	1.00	39.92
1776	C	MET	А	851	60.128	19.901	40.767	1.00	40.11
1777	0	MET	Α	851	60.201	18.982	41.570	1.00	38.44
1778	N	GLN	Α	852	60.894	20.980	40.908	1.00	39.68
1779	CA	GLN	Α	852	61.720	20.958	42.059	1.00	42.72
1780	CB	GLN	Α	852	62.918	21.868	41.882	1.00	41.86
1781	CG	GLN	Α	852	63.758	21.298	40.778	1.00	52.95
1782	CD	GLN	Α	852	65.096	22.010	40.537	1.00	62.78
1783	OE1	GLN	Α	852	65.118	23.232	40.419		60.88
1784	NE2	GLN	Α	852	66.203	21.229	40.419		69.19
1785	C	GLN	A	852	60.804	21.170	43.309		43.28
1786	0	GLN	Α	852	60.916	20.491	44.309		43.36
1787	N .	CYS	Α	853	59.818	22.048	43.242		43.67
1788	CA			853	59.046	22.136	44.454		41.63
1789	CB			853	58.067	23.283	44.417		40.32
1790	SG			853	58.919	24.771	44.088		36.67
1791	C			853	58.330	20.847	44.697		42.12
1792	0			853	57.934	20.608	45.832		42.69
1793	N			854	58.115	20.013	43.675		42.37
1794	CA			854	57.383	18.705	43.926		41.75
1795	CB			854	56.200	18.430	42.946		38.35
1796	CG	TRP			55.327	19.556	42.514		37.67
1797	CD1				54.684	20.557	43.330		35.33
1798		TRP			53.972	21.386			37.18
1799		TRP			54.150	21.016			36.61
1800		TRP			54.937	19.861	41.168		38.28
1801		TRP			55.238	19.302	39.913		35.92
1802		TRP			54.644	19.863	38.774		35.78
1803		TRP			53.886	20.998	38.860		37.11
1804		TRP			53.642	21.597	40.055		36.88
1805	C	TRP			58.249	17.379	44.163		43.48
1806	0			854	57.788	16.232	43.928		40.95
1807	N			855	59.470	17.495	44.694		46.45 47.97
1808	CA			855	60.141	16.215	45.033		
1809	CB			855	61.562		45.421 44.563		49.14 53.78
1810	CG			855	62.300				
1811	CD	GLN	A	855	63.599	16.874	43.944	1.00	57.56

FIGURE 3AI

Α	В	C	D	E	F	G	Н	I	J
1812	OE1	GLN	Δ	855	64.568	17.630	43.788	1.00	58.49
1813	NE2	GLN			63.597	15.574	43.550	1.00	
1814	C	GLN			59.503	15.583	46.185		48.95
1815	0	GLN			59.135	16.279	47.106		48.87
1816	N	GLN			59.417	14.251	46.193		50.70
1817	CA	GLN			58.760	13.603	47.270		51.94
1818	CB	GLN			58.589	12.110	47.270		52.72
1819	CG	GLN			57.987	11.341	48.190		56.53
1820	CD	GLN			56.902	10.378	47.730		67.51
1821	OE1	GLN			57.145	9.159	47.736		70.03
1822	NE2	GLN			55.687	10.921	47.421	1.00	
	C ·	GLN			59.464	13.844	48.587	1.00	
1823					58.839	13.901	49.641		51.92
1824	O N	GLN			60.776	13.901	48.540		53.47
1825	N	GLU			61.455	14.329	49.763		52.94
1826	CA	GLU				13.574	49.763		55.76
1827	CB	GLU			62.751	13.655	49.000		62.73
1828	CG	GLU			63.760	12.357	48.776	1.00	75.13
1829	CD	GLU			64.555 65.792		48.476	1.00	76.93
1830	OE1	GLU				12.306	49.244	1.00	
1831	OE2	GLU			63.876 61.642	11.369	50.058	1.00	
1832	C			857		15.763			50.10
1833	0	GLU			62.330	16.518	49.385		
1834	N	ALA			61.062	16.140	51.162 51.501	1.00	51.40
1835	CA	ALA			60.918	17.553			
1836	CB	ALA			60.376	17.634	52.879		51.91
1837	C	ALA			62.236	18.232	51.481		52.16 49.85
1838	0	ALA			62.369	19.416	51.138 51.999		52.64
1839	N	ALA			63.210	17.476 18.044	52.311		51.38
1840	CA	ALA			64.489	17.114	53.176		52.83
1841	CB C	ALA ALA			65.270 65.149	18.322	51.024		50.59
1842 1843	0	ALA			66.033	19.188	50.921		52.09
1844		ARG			64.677	17.712	49.971		49.07
1845	N CA	ARG			65.287	18.206	48.702		49.33
1846	CB	ARG			65.434	17.117	47.664		49.91
1847	CG	ARG			66.326	15.929	48.098	1.00	
1848	CD	ARG			66.767	14.950	46.979		67.86
1849	NE			860	67.897	15.592	46.310		79.99
1850	CZ	ARG			67.957	15.919	45.009		84.18
1851		ARG			69.035	16.555	44.538		86.30
1852		ARG			66.970	15.583	44.177		86.46
1853	C	ARG			64.642	19.423	48.073		47.17
1854	0	ARG			65.289	20.026	47.190		48.00
1855	N	ARG			63.390	19.778	48.428		43.32
1856	CA	ARG			62.722	20.886	47.710		42.70
1857	CB	ARG			61.279	21.149	48.284		43.25
1858	CG	ARG			60.375	19.925			38.41
1859	CD	ARG			58.992				33.61
1860	NE	ARG			58.563	18.555			39.84
1861	CZ	ARG			57.675		49.776		40.88
1862		ARG			57.041		50.621		47.18
1863		ARG			57.448	16.786	49.809		42.74
1000	-1114			J J L	37.110				

FIGURE 3AJ

А	В	C	D	E	F	G	H	I	J
1864	С	ARG			63.548	22.127	47.982		40.90
1865	0	ARG			64.151	22.197	49.048		45.17
1866	N			862	63.579	23.123	47.135		38.11
1867	CA			862	64.366	24.296	47.443		36.92
1868	CB			862	64.173	25.174	46.248		37.49
1869	CG			862	62.978	24.528	45.479		34.16
1870	CD			862	62.827	23.232	45.881		36.86
1871	C			862	63.565	24.973	48.494		40.68
1872	0			862	62.378	24.679	48.675		38.28
1873	N			863	64.195	25.936	49.155		43.10
1874	CA	LYS			63.626	26.658	50.273		43.38
1875	CB	LYS			64.689	26.934	51.402	1.00	
1876	CG			863	64.809	25.604	52.283		50.07
1877	CD			863	65.801	25.501	53.459		60.38
1878	CE	LYS			65.260	26.211	54.856		67.58
1879	NZ	LYS			66.287	26.302	55.993		63.31
1880	C			863	63.235	27.905	49.612		43.27
1881	0	LYS	Α	863	63.753	28.275	48.476		45.68
1882	N	PHE	Α	864	62.350	28.605	50.290		40.33
1883	CA	PHE	Α	864	61.830	29.779	49.682		37.37
1884	CB	PHE	Α	864	60.731	30.422	50.528		35.46
1885	CG	PHE	А	864	59.441	29.808	50.353		32.57
1886	CD1	PHE	Α	864	58.869	29.099	51.365		34.21
1887	CE1	PHE	Α	864	57.672	28.495	51.231	1.00	31.67
1888	CZ	PHE	Α	864	56.964	28.622	49.961	1.00	31.72
1889	CE2	PHE	Α	864	57.525	29.380	48.954		30.90
1890	CD2	PHE	Α	864	58.743	29.927	49.129		37.14
1891	C	PHE	Α	864	62.874	30.743	49.304		38.42
1892	0	PHE	A	864	62.717	31.509	48.307	1.00	40.96
1893	N	ALA	Α	865	63.875	30.905	50.126	1.00	
1894	CA	ALA	Α	865	64.964	31.837	49.712		40.21
1895	CB	ALA	A	865	66.009	31.987	50.851		40.74
1896	С	ALA	Α	865	65.712	31.328	48.376		39.07
1897	0	ALA	A	865	66.186	32.133	47.578		40.17
1898	N	ASP	А	866	65.855	30.036	48.142		38.13
1899	CA	ASP	Α	866	66.437	29.657	46.850		41.20
1900	CB	ASP	Α	866	66.592	28.205	46.710		42.25
1901	CG	ASP	Α	866	67.356				46.38
1902	OD1	ASP	A	866	68.194	28.328	48.467		45.69
1903	OD2	ASP	Α	866	67.164	26.319	48.255		46.52
1904	С	ASP	А	866	65.471	30.112	45.734		43.03
1905	0	ASP	Α	866	65.895	30.862	44.786		43.71
1906	N	ILE	Α	867	64.154	29.834	45.959		41.85
1907	CA	ILE	A	867	63.161	30.097	44.945	1.00	39.25
1908	CB	ILE	Α	867	61.738	29.686	45.429		40.79
1909	CG1	ILE	A	867	61.715	28.196	45.547	1.00	37.78
1910	CD1	ILE	Α	867	60.587	27.644	46.393	1.00	31.95
1911	CG2	ILE	A	867	60.673	29.978	44.377		40.13
1912	C	ILE	Α	867	63.262	31.517	44.601	1.00	38.15
1913	0	ILE	Α	867	63.383	31.839	43.478	1.00	34.00
1914	N	VAL	Α	868	63.293	32.407	45.587		41.76
1915	CA	VAL	Α	868	63.363	33.826	45.221	1.00	42.24

FIGURE 3AK

A	В	С	D	E	F	G	Н	I	J
1916	СВ	VAL	A	868	63.468	34.646	46.495	1.00	43.37
1917	CG1	VAL	Α	868	63.906	36.180	46.204	1.00	36.83
1918	CG2	VAL			62.167	34.602	47.161	1.00	44.87
1919	С			868	64.595	34.086	44.346	1.00	43.26
1920	0			868	64.566	34.653	43.250	1.00	42.88
1921	N			869	65.709	33.593	44.819	1.00	43.82
1922	CA	SER	Α	869	66.947	33.788	44.034	1.00	45.81
1923	СВ			869	68.135	33.277	44.868	1.00	46.51
1924	OG	SER	Α	869	69.256	32.973	44.081	1.00	55.81
1925	С	SER	Α	869	66.932	33.161	42.595	1.00	43.21
1926	0	SER	Α	869	67.448	33.748	41.646	1.00	45.11
1927	N	ILE	Α	870	66.309	32.041	42.410	1.00	40.48
1928	CA	ILE	Α	870	66.341	31.421	41.081	1.00	41.53
1929	CB	ILE	Α	870	65.721	30.078	41.130	1.00	40.21
1930	CG1	ILE	Α	870	66.726	29.091	41.617	1.00	37.62
1931	CD1	ILE	Α	870	65.913	27.844	42.278	1.00	34.59
1932	CG2	ILE	Α	870	65.227	29.674	39.764	1.00	37.43
1933	C	ILE	Α	870	65.551	32.101	40.057	1.00	41.17
1934	0	ILE	A	870	65.629	31.841	38.862	1.00	45.96
1935	N	LEU	Α	871	64.743	32.960	40.589	1.00	42.32
1936	CA	LEU	Α	871	63.690	33.613	39.857	1.00	39.74
1937	CB	LEU	Α	871	62.477	33.514	40.715	1.00	36.70
1938	CG	LEU	Α	871	61.084	32.948	40.403	1.00	42.57
1939	CD1	LEU	Α	871	61.128	31.584	39.753	1.00	39.10
1940	CD2	LEU	Α	871	60.155	32.800	41.647	1.00	33.43
1941	С	LEU	Α	871	64.073	35.062	39.677	1.00	40.56
1942	0	LEU	Α	871	63.729	35.716	38.685	1.00	39.95
1943	N	ASP	Α	872	64.858	35.566	40.655	1.00	43.30
1944	CA	ASP	Α	872	65.641	36.754	40.333	1.00	45.25
1945	CB	ASP	Α	872	66.270	37.416	41.537	1.00	44.64
1946	CG	ASP	Α	872	65.296	38.054	42.370	1.00	50.39
1947		ASP			64.560	38.981	41.884		58.03
1948	OD2	ASP	Α	872	65.222	37.729	43.584		59.66
1949	C	ASP			66.617	36.467	39.147		42.59
1950	0	ASP			66.673	37.301	38.244		40.36
1951	N	LYS			67.123	35.244	39.030		43.85
1952	CA	LYS			68.158	35.043	37.946		46.85
1953	CB	LYS			68.848	33.639	37.915		47.60
1954	CG	LYS			69.201	33.005			56.65
1955	CD			873					64.86
1956	CE	LYS			71.327				72.42
1957	ΝZ			873	72.948				77.28
1958	C	LYS			67.273	35.234	36.716		45.54
1959	0	LYS			67.554	36.043	35.848		47.71
1960	N	LEU			66.177	34.496	36.670		44.00
1961	CA	LEU			65.345	34.413	35.523		41.76
1962	CB	LEU			64.257	33.510	35.950		42.33
1963	CG	LEU			64.335	32.030	35.627		43.61
1964		LEU			65.728	31.506			39.31
1965		LEU			63.820				40.93
1966	C			874	64.842				41.73
1967	0	LEU	A	874	64.974	36.328	34.103	1.00	40.87

FIGURE 3AL

1968 N ILE A 875	A	В	С	D	E	F	G	Н	I	J
1969	1968	N	TLE	Α	875	64.356	36.539	36.219	1.00	41.36
1970 CB ILE A 875 63.241 38.556 37.045 1.00 41.83 1971 CG1 ILE A 875 61.848 37.830 37.313 1.00 41.11 1973 CG2 ILE A 875 61.307 38.014 38.707 1.00 42.11 1973 CG2 ILE A 875 65.128 39.991 36.768 1.00 43.50 1974 C ILE A 875 65.128 39.991 36.768 1.00 43.50 1975 O ILE A 875 65.128 39.991 36.768 1.00 43.50 1976 N ALA A 876 65.128 39.592 34.357 1.00 42.05 1976 N ALA A 876 66.305 38.724 36.005 1.00 43.68 1977 CA ALA A 876 66.305 38.724 36.005 1.00 47.29 1978 CB ALA A 876 66.366 39.705 36.633 1.00 47.29 1978 CB ALA A 876 68.666 39.705 36.633 1.00 47.39 1980 O ALA A 876 68.349 40.096 33.381 1.00 47.94 1980 O ALA A 876 68.349 40.096 33.381 1.00 49.38 1981 N ALA A 877 67.882 37.894 33.781 1.00 49.67 1982 CA ALA A 877 69.359 36.469 32.485 1.00 47.02 1984 C ALA A 877 69.359 36.469 32.485 1.00 47.02 1984 C ALA A 877 69.359 36.469 32.485 1.00 47.02 1988 C ALA A 877 66.995 35.680 31.364 1.00 48.54 1985 O ALA A 877 66.995 35.680 31.364 1.00 48.54 1986 N PRO A 878 66.165 37.720 31.333 1.00 48.50 1988 CB PRO A 878 64.883 37.290 30.768 1.00 50.31 1989 C PRO A 878 66.369 39.140 31.199 1.00 47.09 1990 C PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.399 39.140 31.199 1.00 47.09 1992 O PRO A 878 66.339 39.140 31.199 1.00 47.09 1993 N ASP A 879 66.313 35.529 27.704 1.00 53.74 1994 CA ASP A 879 66.313 35.529 27.704 1.00 53.47 1995 CB ASP A 879 66.313 35.529 27.704 1.00 53.47 1996 CG ASP A 879 66.313 35.529 27.704 1.00 53.47 1997 ODI ASP A 879 66.311 37.639 25.969 1.00 61.05 1999 C ASP A 879 66.337 34.121 28.137 1.00 49.66 1999 C ASP A 879 66.337 34.121 28.137 1.00 49.66 1999 C ASP A 880 66.494 32.578 30.001 1.00 52.26 2005 C SER A 880 66.494 32.578 30.001 1.00 52.26 2006 O SER A 880 66.494 32.578 30.001 1.00 52.26 2007 N LEU A 881 62.691 32.401 29.788 1.00 44.70 2008 CA LEU A 881 62.691 32.401 29.788 1.00 44.70 2008 CA LEU A 881 61.063 31.708 28.161 1.00 44.09 2008 CA LEU A 881 61.063 31.902 28.406 1.00 46.77 2011 CDI LEU A 881 61.063 31.906 27.480 1.00 46.07 2012 CD2 LEU A 881 61.063 31.909 27.480 1.00 46.07 2013 C L										
1971 CG1 ILE A 875 61.848 37.830 37.313 1.00 41.11 1972 CD1 ILE A 875 61.307 38.014 38.707 1.00 42.11 1973 CG2 ILE A 875 63.128 39.991 36.768 1.00 39.851 1974 C ILE A 875 65.128 39.991 36.768 1.00 39.851 1975 O ILE A 875 64.949 39.592 34.357 1.00 42.05 1976 N ALA A 876 66.305 38.724 36.005 1.00 43.50 1977 CA ALA A 876 66.305 38.724 36.005 1.00 43.50 1978 CB ALA A 876 68.666 39.705 36.633 1.00 47.29 1978 CB ALA A 876 68.666 39.705 36.633 1.00 45.33 1981 N ALA A 876 68.849 40.096 33.381 1.00 49.38 1981 N ALA A 877 67.882 37.894 33.781 1.00 49.67 1982 CA ALA A 877 69.359 36.469 32.485 1.00 47.02 1983 CB ALA A 877 69.359 36.469 32.485 1.00 47.02 1984 C ALA A 877 67.051 36.862 31.723 1.00 48.54 1985 N PRO A 878 66.165 37.720 31.333 1.00 48.54 1986 N PRO A 878 66.165 37.720 31.333 1.00 48.54 1987 CA PRO A 878 64.883 37.290 30.768 1.00 49.52 1988 CB PRO A 878 64.248 38.609 30.314 1.00 49.52 1989 CG PRO A 878 66.369 39.594 30.795 1.00 47.09 1990 CD PRO A 878 66.309 39.594 30.795 1.00 47.09 1991 C PRO A 878 66.309 39.594 30.795 1.00 47.09 1992 C PRO A 878 66.309 39.594 30.795 1.00 50.31 1993 N ASP A 879 66.311 36.423 28.857 1.00 53.47 1994 CA ASP A 879 66.311 36.432 28.857 1.00 53.47 1995 CB ASP A 879 66.313 35.529 27.704 1.00 53.47 1994 CA ASP A 879 66.311 37.639 25.969 1.00 51.52 1999 C ASP A 879 66.311 37.639 25.969 1.00 53.47 1999 C ASP A 879 66.311 37.639 25.969 1.00 53.74 1999 C ASP A 879 66.337 34.121 28.137 1.00 49.60 2000 C ASP A 879 66.337 34.21 28.137 1.00 49.60 2001 N SER A 880 66.687 33.897 29.401 1.00 50.31 2002 CA SER A 880 66.893 32.99 32.357 1.00 52.26 2005 C SER A 880 66.697 33.897 29.401 1.00 50.31 2006 CA SER A 880 66.891 32.401 29.788 1.00 47.09 2007 CB LEU A 881 62.207 33.854 1.00 44.70 2008 CA LEU A 881 62.237 33.897 30.429 1.00 42.64 2010 CG LEU A 881 62.269 32.863 32.997 1.00 44.70 2011 CD1 LEU A 881 61.063 31.708 28.161 1.00 46.07 2012 CD2 LEU A 881 61.063 31.908 27.480 1.00 46.79 2013 C LEU A 881 61.063 31.908 27.480 1.00 46.07 2016 CA LYS A 882 63.66 31.999 22.408 25.100 42.68										
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1974 C ILE A 875 65.128 38.822 35.369 1.00 43.50 1975 O ILE A 875 64.949 39.592 34.357 1.00 42.05 1976 N ALA A 876 66.305 38.724 36.005 1.00 47.29 1978 CA ALA A 876 67.460 39.526 35.543 1.00 47.29 1978 CA ALA A 876 68.686 39.705 36.633 1.00 45.33 1980 O ALA A 876 68.349 40.096 33.381 1.00 49.38 1981 N ALA A 877 67.882 37.448 32.435 1.00 49.67 1982 CA ALA A 877 68.248 37.448 32.485 1.00 48.36 1983 CB ALA A 877 69.359 36.469 32.485 1.00 48.54 1984 C ALA A 877 66.955 35.680 31.364 1.00 48.54 1985 O ALA A 878 66.165 37.20 31.331 1.00 48.54									1.00	39.85
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1976 N ALA A 876 66.305 38.724 36.005 1.00 43.68 1977 CA ALA A 876 67.460 39.526 35.543 1.00 47.29 1978 CB ALA A 876 68.686 39.705 36.633 1.00 47.94 1980 O ALA A 876 68.349 40.096 33.381 1.00 49.38 1981 N ALA A 877 67.882 37.894 33.781 1.00 49.67 1982 CA ALA A 877 68.248 37.448 32.433 1.00 49.67 1983 CB ALA A 877 66.955 36.469 32.485 1.00 47.02 1984 C ALA A 877 66.995 35.680 31.361 1.00 48.54 1985 O ALA A 878 66.165 37.720 31.333 1.00 48.50 1986 N PRO A 878 64.283 37.290 31.361 1.00 48.50 1986 CB PRO A 878 64.283 37.290 31.733 1.00 <td></td> <td></td> <td>ILE</td> <td>Α</td> <td>875</td> <td></td> <td></td> <td>34.357</td> <td>1.00</td> <td>42.05</td>			ILE	Α	875			34.357	1.00	42.05
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1979 C ALA A 876 67.981 39.177 34.150 1.00 47.94 1980 O ALA A 876 68.349 40.096 33.381 1.00 49.38 1981 N ALA A 877 67.882 37.894 33.781 1.00 49.38 1981 CA ALA A 877 68.248 37.448 32.433 1.00 48.36 1983 CB ALA A 877 67.051 36.862 31.723 1.00 48.54 1985 O ALA A 877 67.051 36.862 31.723 1.00 48.54 1985 O ALA A 877 66.995 35.680 31.364 1.00 48.57 1986 N PRO A 878 66.165 37.720 31.333 1.00 48.54 1986 CA PRO A 878 64.883 37.290 30.768 1.00 50.31 1988 CB PRO A 878 64.248 38.609 30.314 1.00 48.50 1987 CA PRO A 878 64.248 38.609 30.314 1.00 48.50 1989 CG PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.309 39.140 31.199 1.00 51.52 1992 O PRO A 878 66.313 35.558 29.329 1.00 51.52 1992 C PRO A 878 66.313 35.558 29.329 1.00 53.47 1995 CB ASP A 879 66.313 35.559 27.704 1.00 53.74 1995 CB ASP A 879 66.313 35.529 27.704 1.00 53.74 1995 CB ASP A 879 66.313 35.529 27.704 1.00 53.74 1995 CB ASP A 879 66.311 37.639 25.969 1.00 53.74 1995 CB ASP A 879 66.311 37.639 25.969 1.00 61.05 1998 OD2 ASP A 879 66.337 34.121 28.137 1.00 52.26 2000 O ASP A 879 66.337 34.121 28.137 1.00 50.31 2002 CA SER A 880 66.687 33.897 29.401 1.00 50.31 2002 CA SER A 880 66.687 33.897 29.401 1.00 50.31 2002 CA SER A 880 66.494 32.578 30.001 1.00 49.70 2003 CB SER A 880 66.867 33.209 32.571 1.00 50.20 2005 C SER A 880 66.869 32.588 31.504 1.00 50.20 2005 C SER A 880 66.869 32.588 31.504 1.00 49.60 2007 N LEU A 881 62.027 33.897 29.401 1.00 49.60 2007 N LEU A 881 62.027 33.897 29.773 1.00 49.66 2007 N LEU A 881 62.027 33.854 31.893 1.00 47.00 2003 CB LEU A 881 62.027 33.854 31.893 1.00 46.70 2003 CB LEU A 881 62.027 33.854 31.893 1.00 46.70 2003 CB LEU A 881 62.027 33.854 31.893 1.00 46.70 2003 CB LEU A 881 62.027 33.854 31.893 1.00 46.70 2001 CC LEU A 881 62.207 33.854 31.893 1.00 46.70 2001 CD LEU A 881 61.063 31.982 29.773 1.00 42.64 2010 CD LEU A 881 61.063 31.982 28.406 1.00 46.70 2015 N LYS A 882 62.872 31.829 26.603 1.00 46.70 2015 N LYS A	1977	CA	ALA	Α	876	67.460	39.526	35.543	1.00	47.29
1980 O ALA A 876 68.349 40.096 33.381 1.00 49.38 1981 N ALA A 877 67.882 37.894 33.781 1.00 49.67 1982 CA ALA A 877 68.248 37.448 32.433 1.00 48.36 1983 CB ALA A 877 69.359 36.469 32.485 1.00 48.54 1985 O ALA A 877 66.995 35.680 31.364 1.00 48.57 1986 N PRO A 878 66.165 37.720 31.333 1.00 48.57 1987 CA PRO A 878 66.165 37.720 31.333 1.00 48.57 1988 CB PRO A 878 64.248 38.609 30.314 1.00 49.52 1989 CG PRO A 878 65.076 39.549 30.795 1.00 48.76 1990 CD PRO A 878 65.005 36.339 29.595 1.00 51.52 <td>1978</td> <td>CB</td> <td>ALA</td> <td>Α</td> <td>876</td> <td>68.686</td> <td>39.705</td> <td>36.633</td> <td>1.00</td> <td>45.33</td>	1978	CB	ALA	Α	876	68.686	39.705	36.633	1.00	45.33
1981 N ALA A 877 67.882 37.894 33.781 1.00 49.67 1982 CA ALA A 877 68.248 37.448 32.435 1.00 48.36 1984 C ALA A 877 67.051 36.862 31.723 1.00 48.54 1985 O ALA A 877 66.995 35.680 31.364 1.00 48.54 1986 N PRO A 878 66.165 37.720 31.333 1.00 48.50 1987 CA PRO A 878 64.883 37.290 30.768 1.00 50.31 1989 CG PRO A 878 64.248 38.609 30.314 1.00 49.52 1989 CG PRO A 878 65.005 36.339 29.595 1.00 47.09 1991 C PRO A 878 65.005 36.339 29.595 1.00 47.09 1991 C PRO A 878 64.080 35.558 29.329 1.00 52.11	1979	С	ALA	Α	876	67.981	39.177	34.150	1.00	47.94
1982 CA ALA A 877 68.248 37.448 32.433 1.00 48.36 1984 C ALA A 877 69.359 36.469 32.485 1.00 47.02 1985 O ALA A 877 66.995 35.680 31.723 1.00 48.54 1986 N PRO A 878 66.165 37.720 31.333 1.00 48.50 1987 CA PRO A 878 66.165 37.720 31.333 1.00 48.50 1989 CG PRO A 878 64.248 38.609 30.314 1.00 49.52 1989 CG PRO A 878 65.076 39.594 30.795 1.00 47.09 1990 CD PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.309 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.300 36.339 29.595 1.00 57.51	1980	0	ALA	Α	876	68.349	40.096	33.381	1.00	49.38
1983 CB ALA A 877 69.359 36.469 32.485 1.00 47.02 1984 C ALA A 877 67.051 36.862 31.723 1.00 48.54 1986 N PRO A 878 66.965 35.680 31.364 1.00 48.87 1987 CA PRO A 878 66.165 37.720 31.333 1.00 48.50 1988 CB PRO A 878 64.883 37.290 30.768 1.00 50.31 1989 CG PRO A 878 65.076 39.594 30.795 1.00 48.76 1990 CD PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.305 36.339 29.595 1.00 52.11 1991 C PRO A 879 66.118 36.423 28.857 1.00 53.74 1994 CA ASP A 879 66.313 35.529 27.704 1.00 53.74	1981	N	ALA	Α	877	67.882	37.894	33.781	1.00	49.67
1984 C ALA A 877 67.051 36.862 31.723 1.00 48.54 1985 O ALA A 877 66.995 35.680 31.364 1.00 48.87 1987 CA PRO A 878 66.965 37.720 31.333 1.00 48.50 1987 CA PRO A 878 64.883 37.290 30.768 1.00 50.31 1989 CG PRO A 878 65.076 39.594 30.795 1.00 48.76 1990 CD PRO A 878 65.005 36.339 29.595 1.00 47.09 1991 C PRO A 878 65.005 36.339 29.595 1.00 52.11 1993 N ASP A 879 66.118 36.423 28.857 1.00 53.47 1994 CA ASP A 879 66.313 35.529 27.704 1.00 53.74 1995 CB ASP A 879 67.561 37.177 26.105 1.00 54.59 <td>1982</td> <td>CA</td> <td>ALA</td> <td>Α</td> <td>877</td> <td>68.248</td> <td>37.448</td> <td>32.433</td> <td>1.00</td> <td>48.36</td>	1982	CA	ALA	Α	877	68.248	37.448	32.433	1.00	48.36
1985 O ALA A 877 66.995 35.680 31.364 1.00 48.87 1986 N PRO A 878 66.165 37.720 31.333 1.00 48.50 1987 CA PRO A 878 64.883 37.290 30.768 1.00 50.31 1988 CB PRO A 878 64.248 38.609 30.314 1.00 49.52 1990 CD PRO A 878 65.076 39.594 30.795 1.00 47.09 1991 C PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.305 36.339 29.595 1.00 51.52 1992 O PRO A 878 64.080 35.558 29.329 1.00 51.52 1992 O PRO A 878 66.313 35.529 27.704 1.00 53.74 1995 CB ASP A 879 67.561 35.840 26.877 1.00 54.59	1983	CB	ALA	Α	877	69.359	36.469	32.485	1.00	47.02
1986 N PRO A 878 66.165 37.720 31.333 1.00 48.50 1987 CA PRO A 878 64.883 37.290 30.768 1.00 50.31 1988 CB PRO A 878 64.248 38.609 30.314 1.00 49.52 1989 CG PRO A 878 65.076 39.594 30.795 1.00 47.09 1991 C PRO A 878 65.005 36.339 29.595 1.00 51.52 1992 O PRO A 878 66.313 35.558 29.329 1.00 52.11 1993 N ASP ASP 66.313 35.529 27.704 1.00 53.74 1994 CA ASP A 879 66.313 35.529 27.704 1.00 54.59 1996 CG ASP A 879 67.426 37.117 26.105	1984	C	ALA	Α	877	67.051	36.862	31.723	1.00	48.54
1987 CA PRO A 878 64.883 37.290 30.768 1.00 50.31 1988 CB PRO A 878 64.248 38.609 30.314 1.00 49.52 1989 CG PRO A 878 65.076 39.594 30.795 1.00 48.76 1990 CD PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 65.005 36.339 29.595 1.00 51.52 1992 O PRO A 878 64.080 35.558 29.329 1.00 52.11 1993 N ASP A 879 66.118 36.423 28.857 1.00 53.47 1994 CA ASP A 879 66.313 35.529 27.704 1.00 53.47 1995 CB ASP A 879 67.561 35.840 26.877 1.00 53.74 1995 CG ASP A 879 66.311 37.639 25.969 1.00 57.55 1999 OD1 ASP A 879 66.311 37.639 25.969 1.00 61.05 1998 OD2 ASP A 879 66.331 37.639 25.969 1.00 61.05 1999 C ASP A 879 66.337 34.121 28.137 1.00 52.26 2000 O ASP A 879 66.66.83 33.243 27.320 1.00 52.16 2001 N SER A 880 66.664 33.243 27.320 1.00 52.16 2001 N SER A 880 66.667 33.897 29.401 1.00 50.31 2002 CA SER A 880 66.494 32.578 30.001 1.00 49.70 2003 CB SER A 880 66.869 32.588 31.504 1.00 49.60 2004 OG SER A 880 65.026 32.063 29.841 1.00 49.60 2005 C SER A 880 65.026 32.063 29.841 1.00 49.60 2006 O SER A 880 64.796 30.895 29.773 1.00 49.60 2007 N LEU A 881 62.691 32.401 29.788 1.00 44.70 2008 CA LEU A 881 62.691 32.401 29.788 1.00 44.70 2009 CB LEU A 881 61.053 35.053 32.335 1.00 42.64 2010 CG LEU A 881 61.053 35.053 32.335 1.00 46.29 2012 CD2 LEU A 881 61.063 31.708 28.161 1.00 46.79 2015 N LYS A 882 63.166 31.996 27.480 1.00 46.05 2016 CA LYS A 882 63.166 31.996 27.480 1.00 46.05 2016 CA LYS A 882 63.166 31.996 27.480 1.00 46.05	1985	0	ALA	Α	877	66.995	35.680		1.00	48.87
1988 CB PRO A 878 64.248 38.609 30.314 1.00 49.52 1989 CG PRO A 878 65.076 39.594 30.795 1.00 48.76 1990 CD PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 66.309 39.140 31.199 1.00 47.09 1992 O PRO A 878 64.080 35.558 29.329 1.00 52.11 1993 N ASP A 879 66.118 36.423 28.857 1.00 53.47 1994 CA ASP A 879 66.313 35.529 27.704 1.00 53.74 1995 CB ASP A 879 67.561 35.840 26.877 1.00 54.59 1996 CG ASP A 879 66.311 37.639 25.969 1.00 61.05 1997 OD1 ASP A 879 66.337 34.121 28.137 1.00 52.26 </td <td>1986</td> <td>N</td> <td>PRO</td> <td>Α</td> <td>878</td> <td>66.165</td> <td>37.720</td> <td>31.333</td> <td></td> <td></td>	1986	N	PRO	Α	878	66.165	37.720	31.333		
1989 CG PRO A 878 65.076 39.594 30.795 1.00 48.76 1990 CD PRO A 878 66.399 39.140 31.199 1.00 47.09 1991 C PRO A 878 65.005 36.339 29.595 1.00 51.52 1992 O PRO A 878 64.080 35.558 29.329 1.00 52.11 1993 N ASP A 879 66.118 36.423 28.857 1.00 53.74 1994 CA ASP A 879 66.313 35.529 27.704 1.00 53.74 1995 CB ASP A 879 66.313 35.529 27.704 1.00 54.59 1996 CG ASP A 879 67.561 35.840 26.877 1.00 54.59 1997 OD1 ASP A 879 66.311 37.639 25.969 1.00 61.05 1998 OD2 ASP A 879 66.337 34.121 28.137 1.00 52.26 2000 O ASP A 879 66.064 33.243 27.320 1.00 52.16 2001 <td>1987</td> <td>CA</td> <td>PRO</td> <td>Α</td> <td>878</td> <td>64.883</td> <td></td> <td></td> <td></td> <td></td>	1987	CA	PRO	Α	878	64.883				
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2017 CB LYS A 882 63.999 32.408 25.172 1.00 42.68						62.872			1.00	44.09
		CB								42.68
2018 CG LYS A 882 63.822 33.855 24.808 1.00 50.65								24.808	1.00	50.65
2019 CD LYS A 882 64.615 34.299 23.548 1.00 57.85	2019	CD	LYS	A	882	64.619	34.299	23.548	1.00	57.85

FIGURE 3AM

A	В	C	D	E	F	G	Н	I	J
2020	CE	LYS	Α	882	66.036	33.711	23.442	1.00	57.83
2021	NZ			882	66.063	32.670	22.379		62.95
2022	C			882	62.712	30.397	25.609		39.93
2023	0			882	62.057		24.624	1.00	
2024	N			883	63.413	29.481	26.255	1.00	36.09
2025	CA			883	63.327	28.070	25.917	1.00	37.39
2026	CB			883	64.642	27.295	26.300	1.00	38.89
2027	OG1	THR	Α	883	65.753	27.896	25.645	1.00	45.06
2028	CG2	THR	Α	883	64.619	25.861	25.703	1.00	34.98
2029	C	THR	Α	883	62.325	27.441	26.760	1.00	37.20
2030	0	THR	Α	883	62.376		27.985	1.00	38.72
2031	N	LEU	Α	884	61.468	26.653	26.136	1.00	36.33
2032	CA			884	60.299	26.154	26.735	1.00	
2033	CB	LEU	Α	884	59.256	26.182	25.688		37.32
2034	CG			884	58.405		25.764	1.00	
2035		LEU			59.168		26.319		40.46
2036		LEU			57.816		24.464		39.93
2037	C			884	60.536		27.146		37.90
2038	0			884	61.439		26.704		37.67
2039	N	ALA			59.766		28.090		40.12
2040	CA	ALA			59.817		28.517		43.23
2041	CB	ALA			59.092	22.789	29.809		40.83
2042	C			885	59.015	22.235	27.462		47.82
2043	0			885	58.130		26.805		48.49
2044	N CA			886	59.249 58.481		27.379 26.460		53.03 57.55
2045 2046	CB			886 886	59.468		25.609		59.17
2046	CG			886	59.801		24.316		66.52
2047		ASP			60.703	19.608	23.581		73.87
2049		ASP			59.214		23.960	1.00	
2050	C			886	57.476	19.113	26.984	1.00	
2051	0			886	57.538		28.103		58.38
2052	N			887	56.511		26.120		62.53
2053	CA			887	55.793		26.245	1.00	63.20
2054	CB	ALA	Α	887	56.793		26.732	1.00	63.87
2055	C	ALA	Α	887	54.506	17.495	27.046	1.00	64.13
2056	0	ALA	Α	887	53.476	18.015	26.589		64.69
4115	01A	ATP	A:	1000	37.488	36.083	52.431		68.23
4116	PA	ATP	A.	1000	38.403		51.393		58.85
4117	02A	ATP	A	1000	39.539	36.819	52.377	1.00	63.08
4118	O3A	ATP	A:	1000	38.307				64.52
4119	PB	ATP	A.	1000	37.326		51.050		65.46
4120		ATP			36.977		52.487		64.98
4121		ATP			38.372		50.835		64.05
4122		ATP			36.030		50.075		61.18
4123	PG	ATP			36.102		48.418		64.66
4124		ATP			37.337		47.992		61.28
4125		ATP			34.842		47.778		53.07
4126		ATP			36.347		47.869		55.85
4127		ATP			37.771				63.69
4128		ATP			36.564				51.19
4129	C4*	ATP	Α.	1000	36.702	38.452	48.619	T.00	48.45

FIGURE 3AN

A	В	С	D	·E		F		G		Н	I	J
4130	04*	ATP	Α1	1000	3	6.838	39	.812	48	.897	1.00	48.02
4131		ATP				7.801		.399		.075		51.30
4132		ATP				8.364		.349		.132		56.06
4133	02*	ATP				7.709		.459		.885		53.71
4134	C3 *	ATP				7.962		.092		.863		56.21
4135		ATP				7.576		.178		.929		56.41
4136	N9	ATP				8.870		.760		.977		48.97
4137	C8	ATP				9.164		.209		.155	1.00	
4138	N7	ATP				0.236		.937		.642		47.18
4139	C5	ATP				0.553		.923		.802		46.85
4140	C6	ATP				1.495		.912		.749		45.05
4141	N6	ATP				2.491		.015		.606		51.47
4141	C4	ATP				9.721		.807		.758		44.98
4142	N3	ATP				9.840		.616		.754		40.18
4144	C2	ATP				0.730		.613		.652		40.86
4145	N1	ATP				1.527		.736		.735	1.00	
4177	0	HOH				4.209				.111		42.77
4178	0	НОН				2.030		.683		.996		37.34
4179		НОН				6.987		.304		.823		48.24
4179	0 ′	НОН				4.445		.848		.354		30.63
		HOH				8.693		.951		.781		33.40
4181 4182	0	HOH				3.619		.688		.907		36.33
		НОН				5.150		.275		.892		38.81
4183	0	НОН				4.293		.454		.291	1.00	
4184	0					6.249		.679		.871		28.41
4185 4186	0	HOH HOH				7.152		.870		.285		44.21
4187		НОН				2.468		.101		.466		34.94
4188	0	НОН				8.705		.579		.068		42.08
4189	0	нон				1.983		.989		.287		43.17
4190	0	нон				0.636		.308		.909		29.96
4191	0	НОН				8.314		.464		.478		53.90
4191	0	НОН				8.592		.555		.508		46.60
4193	0	НОН				4.711		.223		.323	1.00	
4194	0	нон				1.004		.502		.290		43.71
4195		НОН				0.245		.662		.484		39.87
4196	0	нон				3.203		.844		.705		35.11
4197	0	нон				7.565				.482		42.90
4198	0	НОН				1.412						46.40
4199	0	нон				0.121				.919		49.18
4200	0	нон				4.265		.237		.221		38.57
4201	0	нон				5.932		.979		.458		44.49
4202	0	НОН				0.167		.451		.178		43.85
4203	Ö	НОН				3.877		.468		.538		41.56
4204	o	нон				2.331		.960		.402		46.79
4205	0	нон				9.475		.163		.500		41.09
4206	Ö	нон				6.704		.338		.706		32.58
4207	0	НОН				4.910		.079		.822		29.88
4207	0	нон				6.529		.709		.322		38.73
4209	0	нон				4.290		.356		.871		33.86
4210	0	НОН				9.125		.580		.291		52.12
4211	0	нон				0.038		.951		.948		38.53
4212	0	нон				9.032		.142		.076		46.77
	-		_						- '			

FIGURE 3AO

A	В	С	D	E	F	G	Н	I	J
4213	0	нон	Y	338	27.063	12.328	81.741	1.00	49.23
4214	0	HOH	Y	339	43.495	-1.978	101.845	1.00	29.87
4215	0	HOH	Y	340	24.042	11.453	87.471	1.00	41.90
4216	0	HOH	Y	341	28.532	21.817	105.465	1.00	51.38
4217	0	HOH	Y	342	34.250	-2.816	87.557	1.00	40.16
4218	0	HOH	Y	343	61.321	37.753	51.409	1.00	42.73
4219	0	HOH	Y	344	36.839	-8.065	88.494	1.00	47.43
4220	0	HOH	Y	345	36.931	51.353	67.108	1.00	43.87
4221	0	HOH	Y	346	32.133	3.426	74.670	1.00	41.40
4222	0	HOH	Y	347	35.239	-3.830	103.044	1.00	32.29
4223	0	HOH	Y	348	29.414	4.943	100.046	1.00	41.59
4224	0	HOH	Y	349	24.239	20.789	98.495		55.55
4225	0	HOH	Y	350	. 56.249	24.229	27.459	1.00	35.32
4226	0	HOH	Y	351	42.039	36.733		1.00	31.77
4227	0	нон	Y	352	49.598	14.602	89.944		39.22
4228	0	HOH	Y	353	53.086	45.810	55.315	1.00	46.66
4229	0	HOH	Y	354	56.134	28.666	55.481	1.00	37.89
4230	0	HOH	Y	355	63.607	21.585	51.318	1.00	45.92
4231	0	HOH	Y	356	47.007	-0.656	101.802	1.00	39.67
4232	0	HOH	Y	357	56.849	42.289			43.93
4233	0	HOH	Y	358	50.297	45.047	58.166	1.00	37.20
4234	0	HOH	Y	359	28.541	41.183	57.319	1.00	46.64
4235	0	HOH	Y	360	61.669	23.736			46.15
4236	0	HOH	Y	361	46.431	16.691	103.110		35.98
4237	0	HOH	Y	362	43.512	8.970	105.775		36.32
4238	0	HOH	Y	363	62.088	25.972	23.786		38.78
4239	0	HOH	Y	364	64.287	31.187			44.19
4240	0	HOH	Y	365	34.618	30.621			40.96
4241	0	HOH	Y	366	25.281				44.80
4242	0	HOH	Y	367	45.275	20.695	97.308	1.00	46.67

FIGURE 3AP

		•							
Α .	В	С	D	E	F	G	Н	I	J
2057	N	ALA	В	602	61.588	-1.705	97.096	1.00	75.62
2058	CA	ALA	В	602	61.031	-2.970	96.546	1.00	76.68
2059	CB	ALA	В	602	61.665	-3.292	95.199	1.00	76.47
2060	C	ALA	В	602	61.337	-4.080	97.519	1.00	77.44
2061	0	ALA	В	602	61.332	-5.311	97.156	1.00	75.75
2062	N	LYS	В	603	61.635	-3.605	98.744		77.75
2063	CA	LYS	В	603	62.173	-4.417	99.861	1.00	77.56
2064	CB	LYS	В	603	63.425	-3.748	100.411	1.00	78.96
2065	CG			603	63.212	-2.282	100.938	1.00	78.12
2066	CD	LYS		603	62.779	-2.211		1.00	78.99
2067	CE			603	63.952	-2.034		1.00	79.93
2068	NZ	LYS		603	64.536	-0.656		1.00	79.82
2069	С	LYS		603	61.103	-4.418		1.00	76.81
2070	0			603	61.315	-4.798		1.00	75.16
2071	N	PHE	В	604	59.938	-3.975	100.457	1.00	76.03
2072	CA			604	58.711	-3.929		1.00	74.92
2073	CB			604	58.102	-2.575	100.991	1.00	76.05
2074	CG			604	58.700	-1.538		1.00	78.39
2075	CD1			604	58.564	-1.631		1.00	79.39
2076	CE1			604	59.115	-0.671			84.10
2077	CZ			604	59.854	0.395	103.511		81.74
2078	CE2			604	60.017	0.474			82.47
2079	CD2			604	59.448	-0.503	101.312		81.05
2080	C			604	57.783	-5.006	100.707		73.54
2081	0			604	56.553	-4.941		1.00	73.46
2082	N			605	58.368	-6.069		1.00	71.71
2083	CA			605	57.496	-7.068	99.640	1.00	68.96
2084 2085	CB OG1	THR		605 605	57.540	-6.922 -8.191	98.163	1.00	
2086	CG2	THR		605	57.203 58.991	-6.774	97.632 97.722	1.00	71.34 71.15
2087	C			605	57.874	-8.494	99.969		65.74
2088	0			605	59.000	-8.868	99.864		66.65
2089	N			606	56.897	-9.294			61.47
2090	CA			606		-10.702	100.542		56.89
2091	CB	THR		606	55.818		101.234		58.04
2092	OG1	THR		606		-10.407			53.91
2093	CG2	THR				-12.662			56.07
2094	C	THR				-11.402	99.182		55.32
2095	0			606		-11.139	98.285		55.18
2096	N			607		-12.330	99.008		52.87
2097	CA	GLU				-13.077	97.771		48.83
2098	CB	GLU				-13.585	97.546		50.19
2099	CG	GLU				-14.650	96.488		49.52
2100	CD	GLU				-14.069	95.132		53.13

FIGURE 3AQ

A	В	С	D	E	F	G	Н	I	J
2101	OE1	GLU	В	607	59.999	-12.782	95.021	1.00	47.52
2102	OE2	GLU		607	59.708		94.179	1.00	
2103	C	GLU		607	57.128		97.907	1.00	
2104	Ō			607		-14.795	98.940	1.00	45.85
2105	N			608		-14.548	96.865	1.00	47.65
2106	CA			608	55.448	-15.608	97.148	1.00	47.68
2107	CB			608	54.064	-15.132	96.825	1.00	48.07
2108	CG1	ILE	В	608	53.550	-14.230	97.980	1.00	49.31
2109	CD1	ILE	В	608	52.448	-13.233	97.562	1.00	50.75
2110	CG2	ILE	В	608	53.146	-16.282	96.537	1.00	42.03
2111	C	ILE	В	608	55.742	-16.879	96.433	1.00	48.49
2112	0	ILE	В	608	56.251	-16.848	95.356	1.00	47.91
2113	N	HIS	В	609	55.425	-18.022	97.025	1.00	49.63
2114	CA	HIS	В	609	55.656	-19.227	96.270	1.00	51.07
2115	CB	HIS	В	609	56.018	-20.399	97.228	1.00	52.62
2116	CG	HIS	В	609	56.581	-21.599	96.510	1.00	58,.19
2117	ND1	HIS	В	609	55.816	-22.693	96.162	1.00	61.53
2118	CE1	HIS	В	609	56.579	-23.592	95.553	1.00	64.63
2119	NE2	HIS	В	609	57.808	-23.110	95.462	1.00	68.36
2120	CD2	HIS	В	609	57.837	-21.866	96.060		67.33
2121	C	HIS	В	609	54.553	-19.610	95.259		49.78
2122	0	HIS	В	609	53.384	-19.793	95.618		51.06
.2123	N	PRO	В	610		-19.951	94.060		49.31
2124	CA	PRO		610	54.043	-20.289	92.937		48.79
2125	CB			610		-20.868	91.902		47.24
2126	CG	PRO		610	56.241	-20.130	92.245		45.60
2127	CD	PRO		610	56.362	-20.127	93.691		48.27
2128	C	PRO		610	52.968		93.256		47.95
2129	0	PRO		610	51.831	-21.007	92.869		49.54
2130	N	SER		611	53.307	-22.313	93.907		48.59
2131	CA			611		-23.175	94.438		48.44
2132	CB			611		-24.417	95.162		51.57
2133	OG			611		-24.112	96.289		52.63
2134	C			611		-22.460	95.404		47.60 48.97
2135	0	SER		611		-22.969	95.803		
2136	N	CYS		612		-21.290 -20.743	95.872 96.749		46.75 48.06
2137	CA			612					47.86
2138	CB	CYS				-19.740	97.818 98.813		51.39
2139	SG C			612		-20.799 -20.195	96.060		45.77
2140				612 612		-19.972	96.685		45.07
2141	O N			613		-20.011	94.767		44.88
2142	CA	VAL				-19.212	94.037		44.04
2143 2144	CB			613		-18.166	93.300		45.69
2144		VAL				-17.575	92.151		41.35
	CG2	VAL				-17.191	94.320		41.89
2146 2147	CGZ			613		-19.928	93.015		42.53
2147	0	VAL				-20.712	92.308		43.54
2148	N			614		-19.543	92.870		40.71
2149	CA			614		-20.229	91.985		41.54
2151	CB			614		-21.096	92.969		40.51
2152	OG1			614		-22.498	92.671		48.61
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FIGURE 3AR

A	В	С	D	E	F	G	Н	I	J
2153	CG2	THR	В	614	43.817	-20.769	93.108	1.00	44.50
2154	C			614	45.095	-19.149	91.179	1.00	41.38
2155	0			614		-18.144	91.814		42.18
2156	N			615		-19.369	89.853		38.93
2157	CA			615		-18.494	88.956		36.43
2158	CB			615		-18.179	87.724		36.87
2159	CG			615		-17.663	87.956		35.71
2160	CD			615		-17.512	86.727		38.53
2161	NE			615		-18.840	86.152		38.81
2162	CZ			615		-19.126	84.944		38.46
2163	NH1					-20.387	84.635		31.60
2164		ARG				-18.181	84.111		33.51
2165	C			615		-19.117	88.530		37.76
2166	_	ARG				-20.263	88.159		39.62
2166	N .			616		-18.383	88.576		38.21
2167	CA			616		-18.954	88.262		37.39
				616		-18.618	89.472		39.47
2169	CB					-19.563	90.688		43.49
2170	CG			616		-19.363	92.022		50.53
2171	CD			616		-17.701	92.256		48.97
2172		GLN				-17.701	92.230		57.89
2173		GLN							36.84
2174	C			616		-18.178 -18.598	87.047 86.463		32.04
2175	0			616					35.94
2176	N			617		-16.990	86.746 85.725		38.36
2177	CA			617		-16.287			39.22
2178	CB			617		-16.007	86.263 86.233		42.77
2179	CG			617		-14.698			53.79
2180	CD			617		-14.825	86.696		63.68
2181	CE			617 617		-13.466 -12.927	87.025 88.489		63.21
2182	NZ					-12.927	85.316		40.50
2183	C			617		-13.100	86.140		42.28
2184	O			617 618		-14.712	84.039		40.89
2185	N			618		-13.431	83.793		40.18
2186	CA					-13.431	82.385		40.55
2187	CB			618			82.120		44.64
2188		VAL VAL				-11.973 -14.535	82.120		41.80
2189		VAL				-12.346			
				618		-12.485	83.503		39.02
2191	0			619		-12.465	84.559		38.05
2192	N								39.66
2193	CA			619		-10.134 -9.832			40.93
2194	CB			619			86.309		38.06
2195	CG1			619		-9.612	86.979		
2196	CD1			619		-9.252 -11.004	88.632		36.23 40.94
2197	CG2			619		-11.004	87.102		40.94
2198	C			619	40.206	-8.870 -7.812	84.202		
2199	0			619	39.560	-7.812	84.237		42.87
2200	N CA			620	41.393	-8.925 -7.673	83.623		45.17 47.33
2201	CA			620	41.915	-7.673	83.104		50.85
2202	C			620	43.224		82.429		50.85
2203	0			620	43.871				
2204	N	ALA	R	621	43.595	-7.160	81.572	1.00	51.35

FIGURE 3AS

A	В	С	D	E	F	G	Н	I	J
2205	CA	ALA	В	621	44.760	-7.184	80.745	1.00	53.88
2206	СВ			621	44.426	-7.688	79.316		54.10
2207	С			621	45.299	-5.791	80.674	1.00	55.13
2208	0			621	44.828	-4.959	79.886	1.00	57.99
2209	N	GLY	В	622	46.264	-5.589	81.554	1.00	57.03
2210	CA	GLY	В	622	47.168	-4.483	81.562	1.00	59.11
2211	C	GLY	В	622	48.209	-4.562	80.477	1.00	58.66
2212	0	GLY	В	622	48.272	-5.501	79.641	1.00	59.00
2213	N	GLU	В	623	49.057	-3.532	80.510	1.00	59.69
2214	CA	GLU	В	623	50.174	-3.401	79.539	1.00	60.06
2215	CB	GLU	В	623	50.715	-1.953	79.435		61.65
2216	CG	GLU	В	623	51.576	-1.387	80.577	1.00	66.11
2217	CD	GLU	В	623	52.456	-0.197	80.080	1.00	77.25
2218	OE1	GLU	В	623	52.149	0.983	80.464	1.00	79.02
2219	OE2	GLU	В	623	53.437	-0.432	79.272	1.00	79.70
2220	С	GLU			51.309	-4.335	79.842		58.25
2221	0			623	. 52.235	-4.436	79.070		60.16
2222	N			624	51.275	-5.016	80.970		54.74
2223	CA			624	52.410	-5.847	81.262		51.99
2224	CB			624	52.789	-5.730	82.754		51.88
2225	CG			624	53.391	-4.399	83.133		54.02
2226	CD1			624	54.733	-4.102	82.907		55.50
2227	CE1	PHE			55.256	-2.813	83.249		56.20
2228	CZ			624	54.422	-1.780	83.816		56.45
2229	CE2	PHE			53.062	-2.046	84.037		52.77
2230	CD2	PHE			52.556	-3.379	83.686		56.55
2231 2232	С О	PHE PHE			51.975 52.725	-7.269 -8.128	80.865 80.468		50.15
2232	N	GLY			50.672	-7.410	80.863		47.48
2234	CA	GLY			50.054	-8.656	80.601		45.33
2235	C	GLY			48.716	-8.751	81.302		43.78
2236	0	GLY			48.093	-7.765	81.722		43.69
2237	N	GLU				-10.005	81.484		44.33
2238	CA	GLU				-10.291	82.001		43.81
2239	CB	GLU				-11.745	81.695		44.48
2240	CG	GLU				-12.117	80.292		51.57
2241	CD	GLU				-12.312	79.404		61.26
2242	OE1	GLU	В	626	45.469	-11.265	78.940		69.20
2243		GLU				-13.467	79.241		64.36
2244	C	GLU	В	626	46.908	-10.078	83.494	1.00	40.95
2245	0	GLU	В	626	47.921	-10.120	84.202	1.00	41.04
2246	N	VAL	В	627	45.674	-9.798	83.869	1.00	37.16
2247	CA	VAL	В	627	45.186	-9.710	85.213	1.00	35.92
2248	CB	VAL	В	627	44.730	-8.283	85.610	1.00	34.09
2249	CG1	VAL	В	627	44.433	-8.208	87.155	1.00	27.95
2250	CG2	VAL	В	627	45.864	-7.191	85.273	1.00	36.93
2251	C	VAL	В	627	44.123	-10.796	85.471	1.00	35.59
2252	0	VAL				-10.850	84.773		37.84
2253	N	TYR			44.407	-11.644	86.441		31.13
2254	CA	TYR				-12.753			31.63
2255	CB	TYR				-14.055			30.96
2256	CG	TYR	В	628	45.250	-14.532	85.752	1.00	30.76

FIGURE 3AT

A	В	С	D	E	F	G	Н	I	J
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2257		TYR				-14.097	85.486		28.48
2258	CE1			628		-14.488	84.434		30.85
2259	CZ			628		-15.369	83.475		38.38
2260	OH			628		-15.748	82.353		43.82
2261	CE2			628		-15.760	83.588		33.96
2262	CD2			628		-15.354	84.802		34.73
2263	C			628		-12.555	88.305		33.38
2264	0			628		-11.894	89.182		33.26
2265	N			629		-13.240	88.574 89.864		33.61 36.43
2266	CA			629		-13.260 -13.117	89.816		34.99
2267	CB			629 629		-14.031	90.690		42.88
2268	CG CD			629		-13.567	92.036		47.09
2269 2270	CE			629		-14.774	92.959		51.42
2270	NZ			629		-14.774	93.282		38.62
2271	C			629		-14.646	90.264		38.05
2272	0			629		-15.573	89.484		34.96
2273	N			630		-14.773	91.520		39.79
2275	CA			630		-16.017	92.012		40.62
2276	C			630		-16.168	93.499		41.62
2277	0			630		-15.455	94.134		42.67
2278	N			631		-17.122	94.046		42.11
2279	CA			631		-17.424	95.471		40.08
2280	CB			631		-18.782	95.697		39.40
2281	CG			631		-18.772	95.422		36.74
2282	SD			631		-17.481	96.157		46.24
2283	CE			631		-18.103	98.007		44.76
2284	C			631		-17.573	95.862		40.76
2285	0	MET				-18.078	95.080		38.68
2286	N			632		-17.167	97.064	1.00	41.51
2287	CA			632		-17.311	97.497	1.00	43.33
2288	CB	LEU	В	632		-15.967	97.744	1.00	43.33
2289	CG	LEU	В	632		-15.982	98.533	1.00	39.74
2290	CD1	LEU	В	632	49.835	-16.156	97.728	1.00	38.69
2291	CD2	LEU	В	632	48.819	-14.657	99.169	1.00	41.35
2292	C	LEU	В	632	46.389	-18.052	98.813	1.00	47.21
2293	0	LEU	В	632	45.547	-17.737	99.630	1.00	46.45
2294	N	ALA	В	633	47.235	-19.043	98.998	1.00	51.87
2295	CA	ALA	В	633	47.226	-19.803	100.227	1.00	56.44
2296	CB	ALA	В	633	47.668	-21.328	100.004	1.00	56.80
2297	C	ALA	В	633	48.165	-19.045	101.124	1.00	57.40
2298	0	ALA	В	633	49.243	-18.761	100.712	1.00	56.04
2299	N	THR	В	634	47.593	-18.599	102.247	1.00	61.86
2300	CA	THR	В	634	48.165	-17.932	103.448	1.00	65.92
2301	CB	THR	В	634		-16.513		1.00	67.32
2302	OG1	THR	В	634		-16.420			67.54
2303	CG2	THR	В	634	48.373	-15.309	103.123		69.80
2304	C	THR	В	634	47.620	-18.840	104.576		67.85
2305	0	THR	В	634		-19.118			70.48
2306	N	LYS	В	639		-20.684			68.69
2307	CA	LYS	В	639			105.027		66.79
2308	CB	LYS	В	639	42.454	-19.415	105.557	1.00	67.15

FIGURE 3AU

A	В	С	D	E	F	G	Н	I	J
2309	CG	LYS	В	639	42.933	-18.018	106.081	1.00	68.24
2310	CD			639		-17.136			74.03
2311	CE			639			108.280	1.00	79.83
2312	NZ			639	41.868	-18.541	108.918	1.00	77.67
2313	C	LYS	В	639	44.048	-20.001	103.622	1.00	65.00
2314	0	LYS	В	639	45.070	-20.547	103.104	1.00	65.73
2315	N	GLU	В	640	43.302	-19.082	103.006	1.00	60.87
2316	CA	GLU	В	640	43.491	-18.779	101.612	1.00	57.13
2317	CB	GLU	В	640	42.992	-19.919	100.768	1.00	58.15
2318	CG	GLU	В	640	41.495	-19.957	100.494	1.00	60.04
2319	CD	GLU	В	640	41.096	-20.995	99.392	1.00	64.28
2320	OE1	GLU	В	640	39.891	-21.294	99.310	1.00	63.14
2321	OE2	GLU	В	640	41.957	-21.522	98.604	1.00	61.98
2322	C	GLU	В	640	42.667	-17.575	101.332	1.00	54.89
2323	0	GLU	В	640	41.528	-17.402	101.881	1.00	53.30
2324	N	VAL	В	641	43.261	-16.690	100.573	1.00	49.18
2325	CA	VAL	В	641		-15.531		1.00	48.68
2326	CB			641	42.994	-14.411	101.085	1.00	49.50
2327	CG1	VAL	В	641		-14.089	100.811		48.06
2328	CG2	VAL	В	641		-13.327	100.489		57.76
2329	C	VAL	В	641		-15.118	98.866		45.71
2330	0	VAL	В	641		-15.525	97.986		46.28
2331	N	PRO	В	642		-14.483	98.553		43.57
2332	CA	PRO	В	642		-14.052	97.166		40.99
2333	CB	PRO	В	642		-13.620	97.182		40.42
2334	CG			642		-13.154	98.678		41.18
2335	CD			642		-14.358	99.351		42.33
2336	С			642		-12.898	96.773		38.73
2337	0			642		-12.022	97.550		38.87
2338	N			643		-12.896	95.580		36.26
2339	CA			643		-11.916	95.253		35.27
2340	CB			643		-12.558	95.411		35.78
2341	CG1					-12.734	96.921		33.58
2342	CG2	VAL				-13.818	94.815		34.92
2343	C			643		-11.546	93.775		36.64
2344	0			643		-12.389	92.922		38.44
2345	N	ALA				-10.326	93.428		33.63
2346		ALA				-10.046			33.25
2347	CB			644		-8.580	91.626		29.05
2348	C			644		-10.378	91.637		33.38
2349	0			644		-10.129			34.78
2350	N			645		-10.898			34.84
2351	CA			645		-11.220	89.994		34.70
2352	CB			645		-12.634	89.772		36.71 36.62
2353	CG1			645		-13.340	91.011		35.69
2354	CD1			645		-14.627	90.739		36.76
2355	CG2			645		-13.009	89.414		35.66
2356	C			645		-10.663 -11.078	88.716 87.655		33.28
2357	O N			645	48.576	-9.822	88.775		37.62
2358	N CA			646 646		-9.822 -9.156			39.51
2359	CA			646 646					40.50
2360	CB	ПIЭ	0	646	49.392	-7.713	01.334	1.00	10.50

FIGURE 3AV

A	В	С	D	E	F	G	Н	I	J
2361	CG	LYS	В	646	48.112	-6.902	88.103	1.00	43.92
2362	CD			646	48.459	-5.427	88.516	1.00	51.47
2363	CE			646	48.982	-4.629	87.354	1.00	57.30
2364	NZ	LYS	В	646	49.752	-3.453	87.904	1.00	62.15
2365	C			646	50.303	-9.865	87.182	1.00	42.10
2366	0			646	51.198	-10.125	87.959		43.88
2367	N			647		-10.323	85.945	1.00	45.48
2368	CA			647	51.429	-10.990	85.290		46.92
2369	CB			647	50.985	-12.184	84.508	1.00	45.72
2370	OG1			647	49.855	-11.807	83.714	1.00	49.53
2371	CG2			647	50.425	-13.128	85.536	1.00	44.75
2372	C			647	52.160	-10.155	84.313	1.00	47.24
2373	0	THR	В	647	51.699	-9.142	83.797	1.00	48.92
2374	N			648	53.351	-10.596	84.070	1.00	48.96
2375	CA	LEU	В	648	54.249	-9.855	83.227	1.00	50.53
2376	СВ			648	55.590	-9.732	83.968	1.00	49.36
2377	CG	LEU	В	648	56.542	-8.585	83.642	1.00	48.99
2378	CD1	LEU	В	648	58.040	-8.996	83.579	1.00	48.58
2379	CD2	LEU	В	648	56.116	-7.850	82.381	1.00	43.45
2380	С	LEU	В	648	54.374	-10.784	82.043	1.00	51.82
2381	0	LEU	В	648	54.927	-11.893	82.196	1.00	52.19
2382	N	ALA	В	649	53.868	-10.417	80.869	1.00	54.10
2383	CA	ALA	В	649	54.004	-11.362	79.756	1.00	56.21
2384	CB	ALA	В	649		-10.894	78.487	1.00	58.42
2385	C	ALA	В	649	55.446	-11.687	79.395	1.00	
2386	0	ALA	В	649		-10.974	79.740		56.04
2387	N			650		-12.811	78.718	1.00	
2388	CA			650		-13.049	78.140	1.00	
2389	CB			650		-14.433	77.525	1.00	
2390	C			650		-11.965	77.057	1.00	
2391	0			650		-11.510	76.413	1.00	
2392	N			651		-11.595	76.834	1.00	
2393	CA			651		-10.553	75.873	1.00	
2394	C			651	59.312	-9.445	76.746		57.57
2395	0			651	59.712	-8.311	76.347		58.43
2396	N			652 652	59.366 59.573	-9.788 -8.682	78.022 78.940	1.00	58.43 57.59
2397	CA CB				59.435				54.77
2398 2399	CG	TYR		652		-10.134			56.20
2400	CD1			652		-11.415			57.11
2401	CE1			652		-12.382			54.44
2402	CZ			652		-12.044			59.06
2403	OH			652		-13.076	83.485		65.51
2404		TYR				-10.787	82.618		57.44
2405	CD2				61.426		81.867		54.60
2406	C			652	60.713		78.455		57.13
2407	0			652	61.890		78.247		56.27
2408	N			653	60.253		78.165		59.21
2409	CA			653	61.056				61.19
2410	CB			653	60.410			1.00	62.43
2411	OG1			653	58.961	-3.939	78.394	1.00	63.91
2412	CG2	THR	В	653	61.197	-2.732	78.552	1.00	59.49

FIGURE 3AW

A	В	С	D	E	F	G	Н	I	J
2413	С	THR	В	653	62.510	-5.458	78.383	1.00	62.37
2414	0	THR			63.408	-5.096	77.655		63.93
2415	N	ALA			62.748	-6.047	79.537	1.00	65.18
2416	CA	ALA			64.118	-6.339	80.065	1.00	66.92
2417	CB	ALA			65.181	-6.632	78.995	1.00	68.35
2418	C	ALA			64.482	-5.184	80.915		67.15
2419	0	ALA			65.452	-5.259	81.675	1.00	68.11
2420	N	LYS			63.683	-4.123	80.723	1.00	65.70
2421	CA	LYS			63.542	-3.126	81.715	1.00	64.02
2422	CB	LYS			64.033	-1.755	81.277	1.00	64.04
2423	CG	LYS			62.873	-0.760	81.003	1.00	62.73
2424	CD	LYS			62.975	0.659	81.731		66.52
2425	CE	LYS	В	655	61.719	1.600	81.419	1.00	70.62
2426	NZ	LYS	В	655	61.431	3.073	82.018	1.00	71.15
2427	С	LYS			62.035	-3.062	81.945	1.00	64.99
2428	0	LYS			61.594	-2.189	82.707	1.00	65.05
2429	N	ALA			61.184	-3.849	81.273	1.00	65.62
2430	CA	ALA			59.741	-3.683	81.659	1.00	63.59
2431	CB	ALA			58.729	-4.389	80.698	1.00	63.21
2432	C	ALA			59.776	-4.378	83.002	1.00	63.77
2433	0	ALA	В	656	59.045	-4.059	83.953	1.00	65.32
2434	N	ALA			60.688	-5.343	83.081	1.00	62.81
2435	CA	ALA	В	657	60.896	-5.994	84.326	1.00	61.44
2436	CB	ALA	В	657	62.153	-6.830	84.259	1.00	62.87
2437	С	ALA	В	657	60.921	-5.063	85.578	1.00	61.39
2438	0	ALA	В	657	60.315	-5.374	86.615	1.00	60.78
2439	N	VAL	В	658	61.571	-3.906	85.517	1.00	60.99
2440	CA	VAL	В	658	61.752	-3.219	86.804	1.00	60.46
2441	CB	VAL	В	658	62.852	-2.176	86.857	1.00	60.81
2442	CG1	VAL	В	658	64.200	-2.834	86.665	1.00	62.51
2443	CG2	VAL	В	658	62.560	-1.118	85.803	1.00	62.91
2444	C	VAL	В	658	60.583	-2.403	87.005	1.00	59.81
2445	0	VAL	В	658	60.146	-2.289	88.146		58.61
2446	N	ASP	В	659	60.080	-1.838	85.890		58.44
2447	CA	ASP			58.911	-0.960	85.994		57.85
2448	CB	ASP			58.611	-0.274	84.666		58.73
2449	CG	ASP			59.082	1.150	84.657		62.54
2450		ASP			59.986				65.80
2451		ASP			58.612	1.992	85.486		70.42
2452	C	ASP			57.696	-1.717	86.556		55.40
2453	0	ASP			56.889	-1.170	87.285		54.47
2454	N	PHE			57.645	-2.993	86.222		53.30
2455	CA	PHE			56.616	-3.893	86.688		51.47
2456	CB	PHE			56.687	-5.210	85.888		50.03
2457	CG	PHE			55.699	-6.247	86.324		45.78
2458		PHE			54.375	-6.154	85.964		42.78
2459		PHE			53.495	-7.117	86.364		29.42
2460	CZ	PHE			53.919	-8.122	87.106		35.70
2461	CE2	PHE			55.234	-8.230	87.541		34.32
2462	CD2				56.092	-7.299	87.134		41.88
2463	C	PHE			56.809	-4.159			51.98
2464	0	PHE	В	660	55.970	-3.826	88.979	1.00	53.32

FIGURE 3AX

A	В	С	D	E	F	G	Н	I	J
2465	N	LEU	В	661	57.867	-4.818	88.587	1.00	51.16
2466	CA			661	58.052	-4.986	90.025		49.90
2467	CB			661	59.410	-5.608	90.304		50.17
2468	CG			661	59.401	-7.101	89.967		49.47
2469		LEU			60.075	-7.725	91.087		49.31
2470		LEU			58.040	-7.634	90.013		47.87
2471	C			661	58.084	-3.654	90.722		48.85
2472	0			661	57.712	-3.584	91.846		52.10
2473	N			662	58.555	-2.595	90.098		46.78
2474	CA			662	58.683	-1.340	90.803	1.00	44.02
2475	С			662	57.361	-0.929	91.466	1.00	45.84
2476	0			662	57.336	-0.347	92.600	1.00	45.76
2477	N			663	56.258	-1.222	90.753		44.38
2478	CA	GLU	В	663	54.970	-0.787	91.194	1.00	43.00
2479	CB			663	53.843	-1.079	90.191		43.42
2480	CG			663	52.554	-1.313	91.003		48.94
2481	CD			663	51.261	-1.147	90.298		55.99
2482		GLU			50.348	-0.344	90.786		56.46
2483	OE2	GLU		663	51.131	-1.926	89.326	1.00	62.78
2484	C			663	54.735	-1.449	92.490		40.69
2485	0			663	54.243	-0.836	93.429		39.77
2486	N			664	55.147	-2.699	92.549	1.00	41.23
2487	CA			664	54.964	-3.521	93.768		42.51
2488	CB			664	55.361	-4.924	93.525		40.07
2489	C			664	55.811	-2.917	94.871		42.68
2490	0			664	55.438	-2.924	96.042		43.36
2491	N			665	56.960	-2.374	94.476		43.87
2492	CA			665	57.931	-1.819	95.439		43.94
2493	C			665	57.330	-0.667	96.169		43.52
2494	Ō			665	57.462	-0.519	97.381	1.00	44.23
2495	N			666	56.629	0.158	95.425	1.00	42.33
2496	CA			666	55.965	1.280	96.055	1.00	42.70
2497	CB	ILE	В	666	55.513	2.167	94.932	1.00	43.27
2498	CG1	ILE	В	666	56.724	2.800	94.203	1.00	40.47
2499	CD1	ILE	В	666	56.305	3.460	92.869	1.00	45.35
2500	CG2			666	54.692	3.137	95.468	1.00	42.19
2501	C			666	54.729	0.884	96.947	1.00	43.44
2502	0	ILE	В	666	54.624	1.234	98.167	1.00	43.04
2503	N			667	53.817	0.140	96.328	1.00	42.32
2504	CA	MET	В	667	52.569	-0.368	96.938	1.00	42.19
2505	CB			667	51.932	-1.230	95.817	1.00	41.53
2506	CG	MET			51.176	-2.507	96.165	1.00	47.32
2507	SD			667	49.731	-2.572	94.829		52.61
2508	CE			667	50.549	-1.966	93.551	1.00	44.11
2509	C	MET			52.855	-1.095	98.259		40.97
2510	0			667	52.115	-1.057	99.249		40.07
2511	N			668	53.973	-1.762	98.310		41.23
2512	CA			668	54.340	-2.512	99.534		40.60
2513	C	GLY			54.751		100.685		40.90
2514	0	GLY			54.848		101.852		40.12
2515	N			669	54.995		100.355		42.10
2516	CA			669	55.298		101.398		41.36

FIGURE 3AY

A	В	С	D	E	F	G	Н	I	J
2517	СВ	GLN	B	669	55.949	1.743	100.749	1.00	40.50
2518	CG			669	57.369		100.440		44.93
2519	CD			669	57.848	2.816	99.700		53.63
2520	OE1				57.922		100.272	1.00	
	NE2	GLN			58.134	2.617	98.409	1.00	
2521					53.996	1.102			43.35
2522	C	GLN				1.753			45.25
2523	0	GLN		669	54.128				
2524	N	PHE		670	52.769	0.833			41.08
2525	CA			670	51.612		102.134		37.80
2526	CB			670	50.688		101.056		37.43
2527	CG			670	51.446		100.086		36.83
2528	CD1				51.220	2.868	98.724	1.00	
2529	CE1	PHE			51.971	3.676		1.00	
2530	CZ			670	52.941	4.539			43.63
2531	CE2	PHĒ			53078	4.636			39.81
2532	CD2	PHE			52.356		100.563		34.13
2533	C			670	50.888		102.865		35.75
2534	0	PHE	В	670	51.117		102.607		31.50
2535	N	SER	В	671	50.178		103.923		35.37
2536	CA	SER	В	671	49.179	-0.001	104.556		35.63
2537	CB	SER	В	671	49.795	-0.920	105.584	1.00	37.05
2538	OG	SER	В	671	48.754	-1.432	106.452	1.00	35.05
2539	С	SER	В	671	48.009	0.915	105.119	1.00	35.05
2540	0	SER	В	671	48.061	1.604	106.184	1.00	36.76
2541	N	HIS	В	672	46.930	0.915	104.391	1.00	33.56
2542	CA	HIS	В	672	45.871	1.856	104.659	1.00	34.12
2543	CB	HIS	В	672	46.232	3.243	103.989	1.00	32.36
2544	CG	HIS	В	672	45.251	4.288	104.307	1.00	33.02
2545	ND1	HIS	В	672	44.080	4.461	103.586	1.00	33.28
2546	CE1	HIS	В	672	43.406	5.471	104.112	1.00	34.10
2547	NE2	HIS	В	672	44.044	5.886	105.198	1.00	38.41
2548	CD2	HIS	В	672	45.198	5.161	105.333	1.00	38.63
2549	С	HIS			44.633	1.308	104.017	1.00	33.03
2550	0	HIS			44.733	0.644	102.951	1.00	33.41
2551	N	HIS			43.502	1.611	104.635	1.00	30.53
2552	CA	HIS			42.230	1.095	104.299	1.00	31.97
2553	CB	HIS			41.296	1.817	105.206	1.00	30.58
2554	CG	HIS			39.877		105.083	1.00	37.08
2555		HIS			39.369		105.415	1.00	42.49
2556		HIS			38.051		105.241		43.15
2557		HIS			37.690		104.828		31.71
2558		HIS			38.814		104.721		39.22
2559	C	HIS			41.832		102.843		33.87
2560	0	HIS			40.989		102.229		34.38
2561	N	ASN			42.323		102.363		33.75
2562	CA	ASN			41.797		101.126		32.88
2563	CB	ASN			41.166		101.219		30.97
2563 2564	CG	ASN			39.921		101.219		31.43
		ASN			38.806		102.032		30.88
2565 2566									20.74
2566 2567		ASN			40.022		103.273		31.69
2567	C	ASN					100.080		30.93
2568	0	ASN	Þ	0/4	42.730	3.507	99.082	1.00	30.33

FIGURE 3AZ

A	В	С	D	E	F	G	Н	I	J
2569	N	ILE	В	675	43.861	2.055	100.334	1.00	31.51
2570	CA	ILE		675	44.993	1.813	99.460	1.00	30.93
2571	CB	ILE		675	46.273	2.205	100.110		31.44
2572	CG1	ILE	В	675	46.250	3.687	100.454	1.00	28.51
2573	CD1	ILE	В	675	46.340	4.549	99.164	1.00	31.74
2574	CG2	ILE	В	675	47.486	2.026	99.005	1.00	22.20
2575	C	ILE		675	45.052	0.297	99.215		34.26
2576	0	ILE	В	675	44.924	-Ö.515	100.144	1.00	36.44
2577	N	ILE		676	45.186	-0.100	97.964	1.00	34.31
2578	CA	ILE	В	676	44.977	-1.451	97.663	1.00	34.35
2579	CB	ILE		676	44.919	-1.703	96.111	1.00	35.23
2580	CG1	ILE	В	676	44.509	-3.132	95.837	. 1.00	35.18
2581	CD1	ILE	В	676	42.941	-3.264	96.042	1.00	39.25
2582	CG2	ILE		676	46.229	-1.573	95.495	1.00	35.77
2583	С	ILE	В	676	46.143	-2.067	98.326	1.00	34.50
2584	0	ILE		676	47.226	-1.536	98.234	1.00	33.39
2585	N	ARG		677	45.933	-3.239	98.897		33.92
2586	CA	ARG		677	46.961	-3.942	99.559	1.00	33.57
2587	СВ	ARG		677	46.317	-4.719	100.700		32.83
2588	CG	ARG	В	677	47.392	-5.572	101.445	1.00	35.49
2589	CD	ARG		677	46.901	-6.224	102.708		47.46
2590	NE	ARG		677	45.887	-7.206	102.394		52.58
2591	CZ	ARG		677	44.635	-7.100	102.814	1.00	59.96
2592		ARG		677	44.304	-6.024	103.587		55.86
2593	NH2	ARG	В	677	43.742	-8.063	102.463	1.00	56.27
2594	С	ARG	В	677	47.797	-4.926	98.720	1.00	34.17
2595	0	ARG	В	677	47.229	-5.704	97.993	1.00	36.51
2596	N	LEU	В	678	49.115	-4.899	98.837	1.00	33.13
2597	CA	LEU	В	678	50.033	-5.811	98.197	1.00	37.40
2598	CB	LEU	В	678	51.435	-5.236	98.159	1.00	36.36
2599	CG	LEU	В	678	52.397	-6.185	97.415	1.00	42.53
2600	CD1	LEU	В	678	51.911	-6.418	95.980	1.00	35.69
2601	CD2	LEU	В	678	53.852	-5.640	97.304	1.00	41.94
2602	C	LEU	В	678	50.171	-7.067	99.042	1.00	39.09
2603	0	LEU	В	678	50.517	-6.970	100.188	1.00	40.71
2604	N	GLU	В	679	49.836	-8.226	98.507	1.00	41.09
2605	CA	GLU	В	679	49.976	-9.417	99.253	1.00	42.38
2606	CB	GLU	В	679	49.026	-10.474	98.789	1.00	41.41
2607	CG	GLU	В	679	47.562	-10.172	99.081	1.00	45.00
2608	CD	GLU	В	679	47.179	-10.261	100.578	1.00	51.76
2609	OE1	GLU	В	679	47.778	-11.040	101.316	1.00	52.41
2610	OE2	GLU	В	679	46.290	-9.498	101.008	1.00	55.14
2611	C	GLU	В	679	51.363	-9.866	99.118	1.00	42.27
2612	0	GLU	В	679	51.912	-10.278	100.108	1.00	44.77
2613	N	GLY	В	680	51.97 3	-9.623	97.972	1.00	41.28
2614	CA	GLY	В	680	53.256	-10.180	97.623	1.00	41.26
2615	C	\mathtt{GLY}	В	680	53.582	-10.240	96.127	1.00	42.91
2616	0	GLY	В	680	52.890	-9.669	95.349	1.00	42.87
2617	N	VAL	В	681	54.656	-10.893	95.716	1.00	44.63
2618	CA	VAL	В	681	55.060	-10.858	94.316	1.00	47.33
2619	CB	VAL	В	681	56.171	-9.792	93.916	1.00	47.94
2620	CG1	VAL				-8.411	94.202	1.00	48.45
2621		VAL					94.630	1.00	47.53
2622	С	VAL	В	681	55.811	-12.121	94.003	1.00	49.45

FIGURE 3BA

2623	A	В	С	D	E	F	G	Н	I	J
2624 N ILE B 682 55 684 -13.445 92.194 1.00 52.35 2626 CB ILE B 682 56.648 -13.445 92.219 1.00 52.35 2627 CGI ILE B 682 54.614 -14.881 92.219 1.00 42.28 2628 CGI ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.22 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.22 2631 O ILE B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.023 -14.08 90.942 1.00 50.52 2637 O SER B 683	2623	0	VAL	В	681	56.375	-12.823	94.891	1.00	48.56
2625 CA ILE B 682 56.648 -13.445 92.194 1.00 52.57 2626 CB I LE B 682 56.040 -14.781 92.219 1.00 52.57 2627 CG1 ILE B 682 54.614 -14.850 91.771 1.00 54.23 2628 CD1 ILE B 682 53.863 -16.059 92.607 1.00 42.89 2630 C ILE B 682 55.622 -14.986 93.632 1.00 48.84 2630 C ILE B 682 57.528 -13.017 91.033 1.00 54.69 2631 O ILE B 682 57.528 -13.017 91.033 1.00 54.69 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 57.57 2635 OG SER B 683 60.835 -11.648 91.417 1.00 57.57 2635 C SER B 683 60.691 -14.088 90.824 1.00 61.98 2636 C SER B 683 60.691 -14.088 90.824 1.00 61.98 2637 N SER B 683 60.691 -14.088 90.824 1.00 61.98 2638 N ALA B 684 62.404 -15.660 90.662 1.00 65.45 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.45 2641 C ALA B 684 62.404 -15.660 90.662 1.00 65.45 2641 C ALA B 684 62.156 -17.667 89.411 1.00 66.62 2644 CA TYR B 685 59.566 -17.33 88.808 1.00 65.62 2644 CA TYR B 685 59.566 -17.67 89.411 1.00 66.23 2646 C TYR B 685 59.566										
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2629 CG2 ILE B 682 55.622 -14.986 93.632 1.00 48.84 2631 O ILE B 682 57.528 -13.017 91.033 1.00 54.22 2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2633 CA SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.035 -11.648 91.417 1.00 59.27 2635 OG SER B 683 60.835 -11.648 91.417 1.00 60.75 2637 O SER B 683 60.091 -14.088 90.824 1.00 60.75 2637 O SER B 684 60.093 -15.011 91.285 1.00 61.78 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.426 -16.045 92.155 1.00 65.44 2641 C ALA B 684 62.426 -16.045 92.155 1.00 65.44 2641 C ALA B 684 62.156 -17.433 88.808 1.00 65.61 2643 N TYR B 685 59.566 -17.433 88.08 1.00 65.61 <td< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></td<>										
2630 C ILE B 682 57.528 -i3.017 91.033 1.00 54.69 2631 O ILE B 682 57.085 -12.426 89.997 1.00 54.69 2632 N SER B 683 60.026 -12.729 90.672 1.00 59.27 2634 CB SER B 683 60.026 -12.729 90.672 1.00 57.57 2635 OG SER B 683 60.835 -11.648 91.417 1.00 67.57 2636 C SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 62.404 -15.660 90.662 1.00 65.44 2640 CB ALA B 684 62.406 -16.045 92.155 1.00 65.45 2641 C ALA B 684 62.2667 -16.690 89.411 1.00 65.62 2643 N TYR B 685 59.566 -17.667 89.411 1.00 65.62 2643 TYR B 685 59.566 -17.433 88.808 1.00 65.61										
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2632 N SER B 683 58.806 -13.061 91.420 1.00 56.54 2634 CB SER B 683 60.026 -12.729 90.672 1.00 59.27 2635 CG SER B 683 60.835 -11.648 91.417 1.00 67.57 2635 CG SER B 683 60.815 -11.648 91.417 1.00 60.75 2637 O SER B 683 60.691 -14.088 90.824 1.00 60.75 2637 O SER B 683 60.093 -15.011 91.285 1.00 61.98 2638 N ALA B 684 61.921 -14.287 90.467 1.00 64.16 2639 CA ALA B 684 62.404 -15.660 90.662 1.00 65.44 2641 C ALA B 684 62.156 -17.667 89.411 1.00 66.52 2642 O ALA B 684 62.156 -17.667 89.411 1.00 66.62 2643 N TYR B 685 59.566 -17.433 88.080 1.00 65.92 2644 CA TYR B 685 59.5148 -19.196 90.468 1.00 66.23 </td <td></td>										
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2675 N MET B 689 54.593 -12.326 88.964 1.00 49.82										

FIGURE 3BB

A	В	С	D	E	F	G	Н	I	J
2677	СВ	MET	R	689	52 726	-13.198	89.919	1 00	46.09
2678	CG			689		-14.107	88.832		42.85
2679	SD	MET		689		-15.683	89.528		50.11
2680	CE	MET		689		-16.233	88.146		42.03
2681	C	MET		689		-10.876	90.439		44.44
2682	Ö	MET		689		-10.868	91.193		43.66
2683	N	ILE		690	52.546	-9.929	90.420		40.55
2684	CA	ILE		690	52.358	-8.991	91.483		39.05
2685	CB	ILE		690	52.225	-7.585	90.904		41.79
2686	CG1	ILE		690	53.596	-6.955	90.607		40.50
2687	CD1			690	53.501	-5.528	89.890		37.73
2688	CG2			690	51.421	-6.707	91.895	1.00	38.75
2689	С			690	50.932	-9.386	91.986	1.00	
2690	0			690	49.971	-9.343	91.192		36.41
2691	N	ILE	В	691	50.807	-9.788	93.255	1.00	38.28
2692	CA	ILE	В	691		-10.296	93.856	1.00	37.73
2693	СВ	ILE	В	691	49.904	-11.537	94.642	1.00	37.57
2694	CG1	ILE	В	691	50.662	-12.539	93.759	1.00	43.22
2695	CD1	ILE	В	691	49.780	-13.030	92.551	1.00	43.78
2696	CG2	ILE	В	691	48.666	-12.175	95.178	1.00	33.95
2697	C	ILE	В	691	48.965	-9.298	94.809	1.00	37.68
2698	0	ILE	В	691	49.621	-8.935	95.803	1.00	38.31
2699	N	THR	В	692	47.707	-8.901	94.597	1.00	36.61
2700	CA	THR	В	692	47.089	-7.867	95.484	1.00	35.83
2701	CB	THR	В	692	46.777	-6.579	94.767	1.00	34.36
2702	OG1	THR	В	692	46.064	-6.922	93.582	1.00	36.12
2703	CG2	THR	В	692	48.064	-5.799	94.178	1.00	32.38
2704	·C	THR	В	692	45.788	-8.406	96.022	1.00	
2705	0			692	45.333	-9.470	95.601	1.00	
2706	N			693	45.145	-7.663	96.924	1.00	
2707	CA	GLU		693	43.857	-8.165	97.503	1.00	
2708	CB	GLU		693	43.424	-7.317	98.719		33.77
2709	CG	GLU		693	43.251	-5.824	98.385		36.54
2710	CD	GLU		693	42.731	-4.903	99.522		37.60
2711	OE1			693	43.250	-3.736	99.716	1.00	
2712	OE2			693	41.720		100.137	1.00	
2713	C	GLU			42.821	-8.028	96.364		35.07
2714	0	GLU			42.890	-7.067			35.55
2715	N			694		-8.911	96.272		32.10 28.28
2716	CA			694		-8.809			
2717	CB			694		-10.153	94.874 93.769		28.39 32.24
2718	CG			694		-10.217	92.416		28.95
2719	CD1					-9.921 -10.081	91.432		33.82
2720	CE1	TYR				-10.081	91.432		31.62
2721 2722	CZ.			694 694		-10.533	90.899		37.93
2722	CE2			694		-10.655	93.113		35.35
2724	CD2			694		-10.738			35.75
2725	CDZ	TYR				-7.896			28.69
2726	0	TYR				-8.023			28.77
2727	N	MET			39.475				25.99
2728	CA	MET			38.480		94.790		28.69
2,20	CA	1.17.7	ب		20.400	0.010	21.750		

FIGURE 3BC

A	В	С	D	E		F		G		Н	I	J
2729	СВ	MET	В	695	3:	9.057	- 4	1.593	94	.582	1.00	27.01
2730	CG	MET	В	695	4	0.089	- 4	1.121	95	.806	1.00	26.26
2731	SD	MET	В	695	3	9.137	- 4	1.002	97	.332	1.00	29.69
2732	CE	MET	В	695	3	8.140	- 2	2.317	96	.950	1.00	19.49
2733	C	MET	В	695	3	7.337	- 6	5.451	93	.887	1.00	30.89
2734	0	MET	В	695	3	7.371	- 6	5.254	92	.716	1.00	35.87
2735	N	GLU	В	696	3	6.406	- 7	7.188	94	.437	1.00	31.23
2736	CA	GLU	В	696	3	5.369	- 7	7.846	93	.720	1.00	32.82
2737	CB	GLU	В	696	3.	4.419	- 8	3.666	94	.666	1.00	30.79
2738	CG	GLU	В	696	3	3.717	- 7	7.643	95	.469	1.00	38.13
2739	CD	GLU	В	696	3	3.271	- 8	3.107	96	.846	1.00	48.34
2740	OE1	GLU	В	696	3:	2.877	- 9	.291		.897	1.00	61.33
2741	OE2	GLU	В	696	3	3.160	- 7	7.330	97	.803	1.00	43.84
2742	С	GLU	В	696	3-	4.529	- 7	7.028	92	.836	1.00	32.02
2743	0	GLU	₿	696		3.781	- 7	7.625	92	.021	1.00	31.01
2744	N	ASN	В	697	3	4.505	- 5	5.694	92	.943		33.21
2745	CA	ASN	В	697	3	3.694		.999		.904		31.07
2746	CB	ASN	В	697		2.725		1.026		.537		30.83
2747	CG			697		1.440		1.657		.940		34.34
2748		ASN				0.947		5.594		.243		34.99
2749		ASN				0.834		1.156		.055		28.78
2750	C	ASN				4.630		1.265		.926		31.59
2751	0	ASN				4.193		3.413		.103		31.69
2752	N	GLY				5.910		1.526		.990		29.27
2753	CA	GLY				6.768		8.815		.060		29.77
2754	C	GLY				6.882		2.261		.054		29.16
2755	0	GLY				6.746		1.550		.056		31.76
2756	N	ALA				7.160		.773		.888		27.39
2757	CA	ALA				7.387		0.402		.524		26.35
2758	CB	ALA				7.888).293		.086		25.30
2759	C	ALA				6.179).215		.629		27.91
2760	0	ALA				5.168).299		.130		30.28
2761	N	LEU		700		6.280		357		.268		29.27
2762	CA	LEU		700 700		5.121		2.026		.707 .838		32.33 29.30
2763	CB	LEU				5.450		3.069		.301		31.76
2764	CG CD1	LEU LEU		700 700		4.459 3.464		1.089 3.627		.353		30.61
2765 2766						5.145		5.322		. 920		28.14
		LEU						2.671		.617		30.67
2767	C O	LEU				4.449 3.279		2.926		.812		32.59
2768	N							3.092		.584		28.67
2769 2770	CA	ASP ASP				5.175 4.475		3.801		.542		33.44
2771	CB	ASP				5.382		1.505		.575		33.00
2772	CG	ASP				6.230		3.542		.702		38.53
2773		ASP				6.810		2.573		.221		37.75
2774		ASP				6.395		3.751		.440		40.32
2775	C	ASP				3.529		2.791		.837		33.01
2776	0	ASP				2.301		3.048		.715		32.42
2777	N	LYS				4.074		635		.538		30.90
2778	CA	LYS						.568		.960		35.12
2779	CB	LYS				4.186		.548		.449		37.13
2780	CG	LYS				3.542		537		.686		47.55
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FIGURE 3BD

A	В	С	D	E	F	G	Н	I	J
2781	CD	LYS	В	702	34.296	-2.821	83.631	1.00	60.43
2782	CE	LYS		702	33.493	-3.758	82.740		63.91
2783	NZ	LYS		702	34.151	-5.137	82.655		69.98
2784	C	LYS		702	32.158	0.088	85.872	1.00	35.34
2785	0	LYS		702	31.006	-0.038	85.504	1.00	36.22
2786	N		В	703	32.421	-0.020	87.179	1.00	37.97
2787	CA	PHE	В	703	31.403	-0.517	88.060	1.00	34.72
2788	CB	PHE	В	703	31.980	-0.605	89.436	1.00	35.11
2789	CG	PHE	В	703	30.985	-0.877	90.473	1.00	29.25
2790	CD1	PHE	В	703	30.252	-2.115	90.505	1.00	27.25
2791	CE1	PHE	В	703	29.389	-2.361	91.525	1.00	29.92
2792	CZ	PHE	В	703	29.256	-1.467	92.569	1.00	29.83
2793	CE2	PHE	В	703	29.913	-0.313	92.538		29.77
2794	CD2		В	703	30.785	0.001	91.443	1.00	30.63
2795	C	PHE	В	703	30.265	0.452	88.121		36.80
2796	0	PHE	В	703	29.032	0.086	88.137		37.46
2797	N	LEU		704	30.622	1.724	88.157		36.09
2798	CA	LEU		704	29.567	2.730	88.283		35.58
2799	CB	LEU		704	30.162	4.112	88.554		36.04
2800	CG	LEU		704	30.722	4.526	89.921		39.33
2801	CD1			704	31.453	5.870	89.856		39.49
2802	CD2	LEU		704	29.689	4.488	91.097	1.00	39.49
2803	C	LEU		704	28.723	2.859	87.005	1.00	35.48
2804	0	LEU		704	27.545	3.304	87.050	1.00	36.13
2805	N	ARG		705	29.342	2.607	85.865	1.00	
2806	CA	ARG		705	28.645	2.652	84.601		37.41
2807	CB	ARG		705	29.599	2.330	83.433		37.84 34.77
2808	CG	ARG		705	30.260 30.660	3.590 3.455	82.802 81.367		41.95
2809	CD	ARG ARG		705 705	31.988	2.810	81.271		42.52
2810 2811	NE CZ	ARG		705	33.068	3.374	81.792		45.05
2812	NH1	ARG		705	34.261	2.852	81.678		42.04
2813	NH2	ARG		705	32.913	4.565	82.399		40.02
2814	C	ARG		705	27.609	1.598	84.550		40.12
2815	0	ARG		705	26.733	1.639	83.716		43.46
2816	N	GLU		706	27.773	0.561	85.322		41.24
2817	CA	GLU		706	26.916	-0.555	85.216		43.79
2818	СВ			706	27.684	-1.832	85.558	1.00	46.45
2819	CG			706	28.385	-2.583	84.416	1.00	53.31
2820	CD	GLU		706	29.070	-3.871	85.011	1.00	65.10
2821	OE1			706	28.273	-4.757	85.532	1.00	68.07
2822	OE2	GLU	В	706	30.368	-4.034	84.995	1.00	63.05
2823	C	GLU	В	706	25.852	-0.364	86.216	1.00	43.47
2824	0	GLU	В	706	24.864	-1.051	86.164	1.00	45.43
2825	N	LYS	В	707	26.029	0.565	87.117	1.00	43.14
2826	CA	LYS	В	707	25.013	0.851	88.098		44.44
2827	CB	LYS	В	707	25.584	0.449	89.490		46.43
2828	CG	LYS	В	707	26.172	-1.029	89.491		44.84
2829	CD	LYS		707	25.573	-1.880	90.569		43.24
2830	CE	LYS	В	707	25.352	-3.405	90.147		48.65
2831	NZ	LYS		707	24.010	-3.911	90.629		46.05
2832	C	LYS	В	707	24.448	2.319	88.048	1.00	43.63

FIGURE 3BE

A	В	С	D	E	F	G	Н	I	J
2833	0	LYS	В	707	23.968	2.911	89.012	1.00	43.30
2834	N		В	708	24.510	2.886	86.899	1.00	43.40
2835	CA		В	708	24.061	4.208	86.688	1.00	45.41
2836	CB		В	708	23.816	4.329	85.214	1.00	45.17
2837	CG	ASP	В	708	23.571	5.756	84.769	1.00	51.04
2838	OD1	ASP	В	708	23.369	5.861	83.513	1.00	56.65
2839	OD2	ASP	В	708	23.578	6.789	85.536	1.00	50.26
2840	C	ASP	В	708	22.776	4.514	87.400	1.00	46.40
2841	0	ASP	В	708	21.809	3.760	87.256	1.00	48.89
2842	N	GLY	В	709	22.748	5.610	88.155	1.00	45.59
2843	CA	GLY	В	709	21.516	6.076	88.791	1.00	45.68
2844	C	GLY	В	709	21.043	5.454	90.056	1.00	45.97
2845	0	GLY	В	709	20.134	5.987	90.790	1.00	45.98
2846	N	GLU	В	710	21.713	4.355	90.402	1.00	46.33
2847	CA	·GLU	В	710	21.266	3.524	91.498	1.00	44.07
2848	CB	GLU	В	710	21.639	2.091	91.156	1.00	43.37
2849	CG	GLU	В	710	21.240	1.530	89.788	1.00	45.17
2850	CD	GLU		710	21.407	0.012	89.910	1.00	50.33
2851	OE1	GLU		710	21.591	-0.451	91.103	1.00	57.24
2852	OE2	GLU		710	21.522	-0.675	88.894	1.00	45.95
2853	C	GLU		710	21.845	3.640	92.888	1.00	45.39
2854	0	GLU	В	710	21.521	2.760	93.718		47.34
2855	N		В	711	22.760	4.543	93.196		43.13
2856	CA		В	711	23.200	4.589	94.566	1.00	40.55
2857	CB	PHE	В	711	24.679	4.658	94.597	1.00	39.03
2858	CG		В	711	25.276	3.409	94.246	1.00	42.05
2859	CD1		В	711	26.050	3.281	93.108	1.00	38.47
2860	CE1		В	711	26.599	2.064	92.802	1.00	39.65
2861	CZ		В	711	26.275	0.880	93.622	1.00	41.38
2862	CE2	PHE	В	711	25.452	1.062	94.740	1.00	34.06
2863	CD2		В	711	24.989	2.245	95.050	1.00	37.46
2864	C		В	711	22.626	5.863	95.009	1.00	40.79
2865	0		В	711	22.154	6.588	94.204	1.00	41.46
2866	N	SER		712	22.638	6.126	96.287	1.00	42.27 43.06
2867	CA	SER		712	22.217	7.392	96.828	1.00	41.23
2868	CB	SER		712	22.065	7.169	98.297 98.787	1.00	49.09
2869	OG C	SER		712	23.405	7.227			
2870	C	SER		712	23.457 24.613	8.292 7.773	96.753 96.636		43.66 45.02
2871	O N	SER VAL			23.235	9.574	96.953		42.17
2872 2873	CA	VAL			24.207	10.574	96.853		42.95
2874	CB	VAL			23.524	11.961	97.062		44.89
2875	CG1	VAL			24.513	13.096	97.189		44.06
2876		VAL			22.675	12.272	95.826	1.00	
2877	C	VAL		713	25.151	10.328	97.995		43.30
2878	0	VAL			26.361	10.633		1.00	
2879	N	LEU		714	24.607	9.742	99.082		42.36
2880	CA	LEU		714	25.412		100.294		42.34
2881	CB	LEU		714	24.549		101.456		41.80
2882	CG	LEU		714	24.175		102.419		45.27
2883		LEU		714	23.237		103.631		45.36
2884		LEU			25.513		102.995		43.80

FIGURE 3BF

A	В	С	D	E	F	G	Н	I	J
2885	С	LEU	В	714	26.436	8.393	99.951	1.00	40.57
2886	0	LEU	В	714	27.671	8.526	100.117	1.00	40.01
2887	N	GLN		715	25.900	7.402	99.314	1.00	40.78
2888	CA	GLN		715	26.755	6.362	98.870	1.00	40.81
2889	CB	GLN	В	715	25.933	5.288	98.183	1.00	40.42
2890	CG	GLN	В	715	25.177	4.515	99.255	1.00	40.01
2891	CD	GLN	В	715	24.070	3.635	98.723	1.00	44.67
2892	OE1	GLN	В	715	23.548	3.831	97.622	1.00	44.92
2893	NE2	GLN		715	23.716	2.651	99.517	1.00	48.08
2894	C	GLN		715	27.860	6.935	98.036	1.00	39.80
2895	0	GLN		715	29.054	6.675	98.339	1.00	42.92
2896	N	LEU	В	716	27.532	7.760	97.064	1.00	36.73
2897	CA	LEU	В	716	28.556	8.274	96.227	1.00	35.84
2898	CB	LEU		716	27.903	9.036	95.104	1.00	37.36
2899	CG	LEU	В	716	27.084	8.148	94.217	1.00	36.58
2900	CD1	LEU	В	716	26.356	9.177	93.311	1.00	46.24
2901	CD2	LEU	В	716	27.996	7.350	93.371	1.00	37.81
2902	C	LEU	В	716	29.573	9.163	96.975	1.00	36.89
2903	0	LEU	В	716	30.819	9.095	96.782	1.00	36.93
2904	N	VAL	В	717	29.051	10.026	97.831	1.00	37.35
2905	CA	VAL	В	717	29:898	10.905	98.613	1.00	36.10
2906	CB	VAL	В	717	28.967	11.708	99.387	1.00	37.20
2907	CG1	VAL	В	717	29.667	12.776	100.344	1.00	33.48
2908	CG2	VAL	В	717	28.088	12.401	98.375	1.00	38.82
2909	C	VAL	В	717	30.870	10.002	99.410	1.00	38.05
2910	0	VAL	В	717	32.154	10.206	99.454	1.00	37.55
2911	N	GLY		718	30.264	8.952	99.981	1.00	36.80
2912	CA	GLY		718	31.042	8.022	100.772	1.00	33.97
2913	C	GLY		718	32.163	7.457	100.020	1.00	34.81
2914	0	GLY		718	33.349	7.436	100.512	1.00	37.01
2915	N	MET	В	719	31.892	7.099	98.779	1.00	34.31
2916	CA	MET	В	719	33.019	6.609	97.959	1.00	31.67
2917	CB	MET	В	719	32.491	6.176	96.577	1.00	32.74
2918	CG	MET	В	719	31.662	4.841	96.825	1.00	35.62
2919	SD	MET	В	719	30.875	4.103	95.295	1.00	55.32
2920	CE	MET	В	719	30.945	5.495	94.494	1.00	42.34
2921	C	MET		719	34.081	7.610	97.784		30.03
2922 2923	O NT	MET		719	35.279 33.687	7.293 8.847	97.765 97.618		32.08 30.17
2923 2924	N CA	LEU LEU		720 720	34.667	9.890	97.346		33.37
2925	CB	LEU		720	33.986	11.242	96.935		32.33
2926	CG	LEU		720	33.343	11.032	95.575		38.69
2927		LEU		720	32.375	12.150	95.300		38.75
2928		LEU		720	34.427	10.867	94.495		35.80
2929	C	LEU		720	35.489	10.109	98.597		32.85
2930	ō	LEU		720	36.671	10.336			31.06
2931	N	ARG		721	34.809.	10.018	99.755		34.48
2932	CA	ARG		721	35.496		100.996		33.62
2933	СВ	ARG		721	34.472		102.146		35.11
2934	CG	ARG		721	35.051		103.478		34.63
2935	CD	ARG		721	35.575		104.326		39.88
2936	NE	ARG		721	36.004	9.899	105.636	1.00	43.02

FIGURE 3BG

2937 CZ ARG B 721 36.937 9.323 106.397 1.00 45.17 2938 NH1 ARG B 721 37.612 8.271 105.961 1.00 40.58 2939 NH2 ARG B 721 37.213 9.851 107.611 1.00 38.32 2940 C ARG B 721 37.733 9.594 101.591 1.00 31.50 2941 O ARG B 721 37.733 9.594 101.591 1.00 32.33 2942 N GLY B 722 38.6429 7.940 100.919 1.00 30.70 2943 CA GLY B 722 38.555 7.253 99.976 1.00 26.45 2945 O GLY B 722 38.555 7.253 99.976 1.00 26.45 2945 O GLY B 722 38.585 7.253 99.976 1.00 27.04 2946 N ILE B 723 38.180 7.638 98.764 1.00 24.68 2947 CA ILE B 723 38.180 7.638 98.764 1.00 25.40 2949 CGI ILE B 723 38.099 7.129 95.744 1.00 25.40 2949 CGI ILE B 723 38.099 7.129 95.744 1.00 25.40 2949 CGI ILE B 723 38.099 7.129 95.744 1.00 25.42 2955 CDI ILE B 723 39.915 8.818 95.562 1.00 25.42 2955 CDI ILE B 723 40.040 9.056 98.437 1.00 27.97 2953 O ILE B 723 40.040 9.056 98.437 1.00 27.97 2955 CA ALA B 724 40.055 11.203 99.382 1.00 31.44 2956 CB ALA B 724 40.055 11.203 99.382 1.00 31.42 2957 C ALA B 724 40.994 10.756 100.578 1.00 32.43 2958 O ALA B 724 40.994 10.756 100.578 1.00 32.43 2956 CB ALA B 724 40.994 10.756 100.578 1.00 32.43 2956 CB ALA B 724 40.994 10.756 100.578 1.00 32.43 2956 CB ALA B 724 40.994 10.756 100.578 1.00 32.43 2956 CB ALA B 724 40.994 10.756 100.578 1.00 32.43 2956 CB ALA B 724 40.994 10.756 100.578 1.00 32.43 2956 CB ALA B 725 40.599 9.778 101.386 1.00 32.15 2960 CA ALA B 725 40.599 9.778 101.386 1.00 32.45 2966 CA ALA B 725 40.599 9.786 100.366 1.00 32.65 2966 CA ALA B 725 44.656 1.099 99.853 1.00 33.49 2966 CA ALA B 725 44.651 10.999 97.853 1.00 33.06 2968 N MET B 727 44.051 10.999 97.853 1.00 33.69 2966 CA ALA B 725 44.651 10.999 97.853 1.00 33.40 2972 SD MET B 727 44.051 10.999 97.853 1.00 33.40 2972 SD MET B 727 44.051 10.999 97.853 1.00 33.40 2973 CB MET B 727 44.051 10.999 97.853 1.00 33.40 2973 CB MET B 727 45.618 10.999 97.853 1.00 33.40 2973 CB MET B 727 45.618 10.999 97.853 1.00 33.40 2973 CB MET B 727 45.618 10.999 97.853 1.00 33.40 2973 CB MET B 727 45.618 10.999 97.853 1.00 33.40 2973 CB MET B 727 45.618 10.999 97.853 1.00 33.40 297	A	В	C	D	E	F	G	Н	I	J
2938 NH1 ARG B 721 37.612 8.271 105.961 1.00 40.58 2940 C ARG B 721 37.213 9.851 107.611 1.00 31.50 2941 O ARG B 721 36.678 9.202 101.170 1.00 32.33 2942 N GLY B 722 36.429 7.940 100.919 1.00 24.89 2944 C GLY B 722 39.751 7.161 100.307 1.00 24.68 2945 O GLY B 722 39.751 7.161 100.307 1.00 24.68 2945 O ILE B 723 38.180 7.638 98.764 1.00 25.69 2949 CG1 ILE B 723 38.095 7.129 95.744 1.00 22.540 2951 CG2 ILE B 723 38.099	2937	CZ	ARG	В	721	36.937	9.323	106.397	1.00	45.17
2939 NH2 ARG B 721 37.213 9.801 107.611 1.00 38.32 2940 C ARG B 721 36.678 9.202 101.170 1.00 31.50 2942 N GLY B 722 36.429 7.940 100.919 1.00 30.70 2943 C GLY B 722 37.450 6.885 100.918 1.00 24.89 2944 C GLY B 722 38.180 7.638 98.764 1.00 24.68 2945 O ILE B 723 38.180 7.638 98.764 1.00 25.40 2948 CB ILE B 723 38.099 7.129 95.744 1.00 25.40 2948 CG ILE B 723 38.099 7.129 95.744 1.00 25.40 2951 CG2 ILE B 723 39.915										
2940 C ARG B 721 36.678 9.202 101.170 1.00 31.50 2941 O ARG B 721 37.783 9.594 101.591 1.00 32.33 2943 CA GLY B 722 36.429 7.940 100.919 1.00 24.89 2944 C GLY B 722 38.535 7.253 99.976 1.00 26.45 2946 N ILE B 723 38.180 7.638 98.764 1.00 25.69 2947 CA ILE B 723 38.180 7.638 98.764 1.00 25.69 2948 CB ILE B 723 38.728 8.341 96.509 1.00 25.69 2949 CG1 ILE B 723 38.089 7.129 95.744 1.00 23.38 2950 CDI ILE B 723 39.915 8.818 95.562 1.00 27.72 2951 CG2 ILE B 723 39.915 8.818 95.562 1.00 27.97 2953 O ILE B 723 39.915 8.818 1.00 27.97 2955 CA ALA B 724 49.932 <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>										
2941 O ARG B 721 37.783 9.594 101.591 1.00 32.33 2943 CA GLY B 722 36.429 7.940 100.919 1.00 30.70 2944 C GLY B 722 37.450 6.885 100.918 1.00 26.45 2945 O GLY B 722 39.751 7.161 100.307 1.00 27.04 2946 N ILE B 723 38.180 7.638 89.7641 1.00 25.69 2948 CB ILE B 723 38.788 8.341 96.509 1.00 25.69 2948 CB ILE B 723 38.089 7.129 95.744 1.00 23.38 2950 CDI ILE B 723 38.089 7.129 95.744 1.00 25.49 2951 CGI ILE B 723 39.915 8.818 95.562 1.00 27.70 2951 CG ILE B 723 40.040 9.056 84.47 1.00 27.72 2952 C ILE B 723 40.040 9.056 84.37 1.00 27.72 2955 CA ALA B 724 40.905 1.00 30.09 1.00 30.09 29										
2942 N GLY B 722 36.429 7.940 100.919 1.00 30.70 2943 C GLY B 722 37.450 6.885 100.918 1.00 24.89 2945 O GLY B 722 39.751 7.161 100.307 1.00 27.04 2946 N ILE B 723 38.180 7.638 98.764 1.00 24.68 2947 CA ILE B 723 38.180 7.638 97.861 1.00 25.40 2948 CB ILE B 723 38.089 7.129 95.744 1.00 25.40 2949 CGI ILE B 723 36.956 7.550 94.656 1.00 17.00 2950 CDI ILE B 723 39.915 8.818 95.562 1.00 27.97 2951 CG2 ILE B 723 39.915 8.818 95.562 1.00 27.97 2953 O ILE B 723 40.040 9.056 98.437 1.00 27.97 2954 N ALA B 724 39.321 10.112 98.878 1.00 27.72 2955 CA ALA B 724 49.3321 10.012 98.878 1.00 32.43 2956 CB ALA B 724 40.055 11.203			ARG	В						
2943 CA GLY B 722 37.450 6.885 100.918 1.00 24.89 2944 C GLY B 722 38.535 7.253 99.976 1.00 26.45 2946 N ILE B 723 38.180 7.638 98.764 1.00 24.68 2947 CA ILE B 723 39.285 7.928 97.861 1.00 25.69 2948 CB ILE B 723 38.089 7.129 95.744 1.00 23.38 2949 CGI ILE B 723 36.956 7.550 94.656 1.00 17.00 23.38 2950 CDI ILE B 723 36.956 7.550 94.656 1.00 27.02 2951 CG2 ILE B 723 40.040 9.056 98.437 1.00 27.97 2952 C ILE B 723 40.040 9.056 98.437 1.00 27.97 2953 O ILE B 723 40.040 9.056 98.437 1.00 27.97 2954 N ALA B 724 39.321 10.112 98.878 1.00 27.72 2955 CA ALA B 724 40.055 11.203 99.382 1.00 31.14 2956 CB ALA B 724 40.055 11.203 99.382 1.00 31.14 2957 C ALA B 724 40.055 11.203 99.382 1.00 31.04 2958 A ALA B 724 40.055 11.203 99.382 1.00 31.49 2955 CA ALA B 724 40.994 10.756 100.578 1.00 33.49 2956 CB ALA B 725 40.599 9.778 101.386 1.00 37 1.00 36.23 2959							7.940	100.919		
2944 C GLY B 722 38.535 7.253 99.976 1.00 26.45 2945 O ILE B 723 39.751 7.161 100.307 1.00 27.04 2947 CA ILE B 723 38.180 7.638 98.764 1.00 25.69 2948 CB ILE B 723 38.788 8.341 96.509 1.00 25.40 2949 CGI ILE B 723 38.089 7.129 95.744 1.00 23.38 2950 CDI ILE B 723 36.995 7.550 94.656 1.00 17.00 2951 CG2 ILE B 723 40.040 9.056 98.437 1.00 27.72 2953 O ILE B 723 40.040 9.056 98.437 1.00 27.72 2954 N ALA B 724 40.055 11.203 99.382 1.00 27.72 2955 CA ALA B 724 40.994 10.756 100.578 1.00 32.43		CA	GLY	В					1.00	24.89
2946 N ILE B 723 38.180 7.638 98.764 1.00 24.68 2947 CA ILE B 723 39.285 7.928 97.861 1.00 25.69 2949 CGI ILE B 723 38.089 7.129 95.744 1.00 23.38 2950 CDI ILE B 723 36.956 7.550 94.656 1.00 27.92 2951 CG ILE B 723 39.915 88.818 95.562 1.00 27.97 2953 O ILE B 723 41.273 9.063 98.412 1.00 27.79 2953 O ILE B 724 39.9321 10.112 98.878 1.00 27.79 2955 CA ALA B 724 40.095 11.203 99.877 1.00 30.09 2956 CB ALA B 724 40.994	2944	C			722	38.535	7.253	99.976	1.00	26.45
2947 CA ILE B 723 39.285 7.928 97.861 1.00 25.69 2948 CB ILE B 723 38.728 8.341 96.509 1.00 25.40 2949 CGI ILE B 723 38.089 7.129 95.744 1.00 23.38 2950 CDI ILE B 723 36.956 7.550 94.656 1.00 25.42 2952 C ILE B 723 40.040 9.056 98.437 1.00 27.77 2953 O ILE B 723 40.040 9.063 98.412 1.00 27.72 2954 N ALA B 724 39.321 10.112 98.878 1.00 27.72 2955 CA ALA B 724 40.055 11.203 99.382 1.00 31.14 2956 CB ALA B 724 40.955 11.203 99.387 1.00 30.09 2957 C ALA B 725 40.959 10.0576 100.578 1.00 32.43 2958 O ALA B 725 40.994 10.756 100.578 1.00 <td>2945</td> <td>0</td> <td>GLY</td> <td>В</td> <td>722</td> <td>39.751</td> <td>7.161</td> <td>100.307</td> <td>1.00</td> <td>27.04</td>	2945	0	GLY	В	722	39.751	7.161	100.307	1.00	27.04
2948 CB ILE B 723 38.728 8.341 96.509 1.00 25.40 2949 CG1 ILE B 723 38.089 7.129 95.744 1.00 23.38 2950 CD1 ILE B 723 36.956 7.550 94.656 1.00 25.42 2952 C ILE B 723 40.040 9.056 98.437 1.00 27.97 2953 O ILE B 723 41.273 9.063 98.412 1.00 27.97 2955 CA ALA B 724 40.055 11.203 99.382 1.00 27.72 2955 CA ALA B 724 40.055 11.203 99.382 1.00 30.14 2955 CA ALA B 724 40.0994 10.756 100.578 1.00 30.43 2957 C ALA B 724 40.994 10.756 100.578 1.00 30.43 2959 N ALA B 725 40.599 9.778 101.386 1.00 32.43 <td>2946</td> <td>N</td> <td>ILE</td> <td>В</td> <td>723</td> <td>38.180</td> <td>7.638</td> <td>98.764</td> <td>1.00</td> <td>24.68</td>	2946	N	ILE	В	723	38.180	7.638	98.764	1.00	24.68
2949 CG1 ILE B 723 36.956 7.550 94.656 1.00 27.00 2951 CG2 ILE B 723 36.956 7.550 94.656 1.00 17.00 2952 C ILE B 723 40.040 9.056 98.437 1.00 27.97 2953 O ILE B 723 41.273 9.063 98.412 1.00 29.92 2955 CA ALA B 724 39.321 10.112 98.878 1.00 27.97 2955 CA ALA B 724 40.055 11.203 99.837 1.00 30.09 2957 C ALA B 724 42.102 11.293 100.707 1.00 30.243 2957 C ALA B 724 42.102 11.293 100.757 1.00 30.09 2957 C ALA B 725 40.599	2947	CA	ILE	В	723	39.285	7.928	97.861	1.00	25.69
2950 CD1 ILE B 723 36.956 7.550 94.656 1.00 17.00 2951 CG2 ILE B 723 39.915 8.818 95.562 1.00 25.42 2952 C ILE B 723 40.040 9.056 98.437 1.00 27.97 2953 O ILE B 724 41.273 9.063 98.412 1.00 29.72 2955 CA ALA B 724 39.321 10.112 98.878 1.00 27.72 2955 CA ALA B 724 40.055 11.203 99.382 1.00 31.04 2957 C ALA B 724 40.994 10.756 100.578 1.00 32.43 2958 O ALA B 725 40.599 9.778 101.386 1.00 32.15 2959 N ALA B 725 40.599 9.778 101.386 1.00 32.15 2961 CB ALA B 725 42.563 8.568 103.649 1.00 31.6	2948	CB	ILE	В	723	38.728	8.341	96.509	1.00	25.40
2951 CG2 ILE B 723 39.915 8.818 95.562 1.00 25.42 2952 C ILE B 723 40.040 9.056 98.437 1.00 27.97 2953 N ALA B 724 39.321 10.112 98.878 1.00 27.72 2955 CA ALA B 724 40.055 11.203 99.382 1.00 31.14 2956 CB ALA B 724 40.055 11.203 99.382 1.00 31.14 2957 C ALA B 724 40.994 10.756 100.578 1.00 30.09 2957 C ALA B 725 40.994 10.756 100.578 1.00 32.43 2959 N ALA B 725 40.599 9.778 101.386 1.00 32.15 2969 CA ALA B 725 40.599 9.778 101.386 1.00 33.49 2961 CB ALA B 725 40.599 9.778 101.386 1.00 33.49 <td>2949</td> <td>CG1</td> <td>ILE</td> <td>В</td> <td>723</td> <td>38.089</td> <td>7.129</td> <td>95.744</td> <td>1.00</td> <td>23.38</td>	2949	CG1	ILE	В	723	38.089	7.129	95.744	1.00	23.38
2952 C ILE B 723 40.040 9.056 98.437 1.00 27.97 2953 O ILE B 723 41.273 9.063 98.412 1.00 29.92 2954 N ALA B 724 40.055 11.203 99.382 1.00 31.14 2956 CB ALA B 724 40.055 11.203 99.382 1.00 31.14 2957 C ALA B 724 40.994 10.756 100.578 1.00 32.43 2959 N ALA B 725 40.599 9.778 101.386 1.00 32.15 2960 CA ALA B 725 40.599 9.778 101.386 1.00 33.49 2961 CB ALA B 725 40.465 8.568 103.649 1.00 31.16 2961 CB ALA B 725 42.563 8.658 102.180 1.00 33.06 2963 O ALA B 725 42.407 7.837 101.34 1.00 29.5 <td< td=""><td>2950</td><td>CD1</td><td>ILE</td><td>В</td><td>723</td><td>36.956</td><td>7.550</td><td>94.656</td><td>1.00</td><td>17.00</td></td<>	2950	CD1	ILE	В	723	36.956	7.550	94.656	1.00	17.00
2953 O ILE B 723	2951	CG2	ILE	В	723	39.915	8.818	95.562	1.00	25.42
2954 N ALA B 724 39.321 10.112 98.878 1.00 27.72 2955 CA ALA B 724 40.055 11.203 99.382 1.00 31.14 2957 C ALA B 724 40.994 10.756 100.578 1.00 30.09 2957 C ALA B 724 40.994 10.756 100.578 1.00 32.43 2959 N ALA B 725 40.599 9.778 101.386 1.00 32.15 2960 CA ALA B 725 40.599 9.778 101.386 1.00 32.15 2961 CB ALA B 725 40.465 8.568 103.649 1.00 33.04 2961 CB ALA B 725 42.653 8.658 102.180 1.00 33.06 2963 O ALA B 726 42.407 7.837 101.134 1.00 29.85 2964 N GLY B 726 43.519 7.036 100.688 1.00 36.99 <td>2952</td> <td>С</td> <td>ILE</td> <td>В</td> <td>723</td> <td>40.040</td> <td>9.056</td> <td></td> <td>1.00</td> <td>27.97</td>	2952	С	ILE	В	723	40.040	9.056		1.00	27.97
2955 CA ALA B 724 40.055 11.203 99.382 1.00 31.14 2956 CB ALA B 724 39.092 12.388 99.837 1.00 30.09 2957 C ALA B 724 40.994 10.756 100.578 1.00 32.43 2958 O ALA B 725 40.599 9.778 101.386 1.00 32.43 2959 N ALA B 725 40.599 9.778 101.386 1.00 33.49 2961 CB ALA B 725 40.465 8.568 103.649 1.00 31.16 2962 C ALA B 725 42.563 8.568 102.180 1.00 33.06 2963 O ALA B 725 42.563 8.568 102.180 1.00 33.06 2965 CA GLY B 726 42.407 7.837 101.134 1.00 29.85 2965 CA GLY B 726 43.519 7.036 100.688 1.00 31.48 <td>2953</td> <td>0</td> <td>ILE</td> <td>В</td> <td>723</td> <td>41.273</td> <td>9.063</td> <td>98.412</td> <td>1.00</td> <td>29.92</td>	2953	0	ILE	В	723	41.273	9.063	98.412	1.00	29.92
2956 CB ALA B 724 39.092 12.388 99.837 1.00 30.09 2957 C ALA B 724 40.994 10.756 100.578 1.00 32.43 2958 N ALA B 725 40.599 9.778 101.386 1.00 32.15 2960 CA ALA B 725 41.367 9.437 102.613 1.00 33.49 2961 CB ALA B 725 40.465 8.568 103.649 1.00 31.16 2962 C ALA B 725 42.563 8.658 102.180 1.00 33.06 2963 O ALA B 726 43.630 8.759 102.838 1.00 36.69 2964 N GLY B 726 43.519 7.036 100.688 1.00 29.85 2967 O GLY B 726 44.531 8.080 100.151 1.00 32.07 2969 CA	2954	N	ALA	В	724	39.321		98.878		
2957 C ALA B 724	2955	CA	ALA	В	724	40.055	11.203	99.382		
2958 O ALA B 724 42.102 11.293 100.707 1.00 36.23 2959 N ALA B 725 40.599 9.778 101.386 1.00 32.15 2960 CA ALA B 725 41.367 9.437 102.613 1.00 33.49 2961 CB ALA B 725 40.465 8.568 103.649 1.00 31.16 2962 C ALA B 725 42.563 8.658 102.180 1.00 33.06 2964 N GLY B 726 42.407 7.837 101.134 1.00 29.85 2965 CA GLY B 726 43.519 7.036 100.688 1.00 26.93 2966 C GLY B 726 44.531 8.080 100.151 1.00 31.48 2967 O GLY B 726 45.699 7.946 100.370 1.00 32.07 2969 CA	2956	CB	ALA	В	724	39.092				
2959 N ALA B 725 40.599 9.778 101.386 1.00 32.15 2960 CA ALA B 725 41.367 9.437 102.613 1.00 33.49 2961 CB ALA B 725 40.465 8.568 103.649 1.00 31.16 2962 C ALA B 725 42.563 8.658 102.180 1.00 33.06 2963 O ALA B 725 43.630 8.759 102.838 1.00 29.85 2965 CA GLY B 726 42.407 7.837 101.134 1.00 29.85 2966 C GLY B 726 43.519 7.036 100.688 1.00 26.93 2966 C GLY B 726 44.531 8.080 100.151 1.00 31.48 2967 O GLY B 726 45.699 7.946 100.370 1.00 28.56 2968 N MET B 727 44.033 9.136 99.451 1.00 31.48 2967 O GLY B 727 44.033 9.136 99.451 1.00 32.07 2979 CB MET B 727 44.051 10.999 97.853 1.00 31.54 2972 SD MET B 7	2957	C	ALA	В	724	40.994	10.756			
2960 CA ALA B 725 41.367 9.437 102.613 1.00 33.49 2961 CB ALA B 725 40.465 8.568 103.649 1.00 31.16 2962 C ALA B 725 42.563 8.658 102.180 1.00 33.06 2963 O ALA B 725 43.630 8.759 102.838 1.00 36.69 2964 N GLY B 726 42.407 7.837 101.134 1.00 29.85 2965 CA GLY B 726 43.519 7.036 100.688 1.00 26.93 2966 C GLY B 726 44.531 8.080 100.151 1.00 31.48 2967 O GLY B 726 44.531 8.080 100.151 1.00 31.48 2968 N MET B 727 44.033 9.136 99.451 1.00 32.07 2969 CA MET B 727 44.899 10.121 98.846 1.00 33.40 2971 CG MET B 727 44.899 10.121 98.846 1.00 33.40 2971 CG MET B 727 44.899 10.121 98.846 1.00 33.40 2971 CG MET B 727 44.815 10.999 97.853 1.00 33.54 2972 SD MET B 727 45.180 9.612 95.806 1.00 33.05 2973 CE MET B 727 46.410 10.934 95.492 1.00 31.10 2975	2958	0								
2961 CB ALA B 725 40.465 8.568 103.649 1.00 31.16 2962 C ALA B 725 42.563 8.658 102.180 1.00 33.06 2963 O ALA B 725 43.630 8.759 102.838 1.00 36.69 2964 N GLY B 726 42.407 7.837 101.134 1.00 29.85 2965 CA GLY B 726 43.519 7.036 100.688 1.00 26.93 2966 C GLY B 726 44.531 8.080 100.151 1.00 31.48 2967 O GLY B 726 45.699 7.946 100.370 1.00 28.56 2968 N MET B 727 44.031 9.136 99.451 1.00 32.07 2969 CA MET B 727 44.899 10.121 98.846 1.00 32.07 2970 CB MET B 727 44.051 10.999 97.853 1.00 33.40 2971 CG MET B 727 43.815 10.423 96.365 1.00 31.54 2972 SD MET B 727 45.180 9.612 95.806 1.00 35.66 2973 CE MET B 727 46.441 10.934 95.492 1.00 31.92 2974 C MET B 727 46.441 10.93	2959	N								
2962 C ALA B 725 42.563 8.658 102.180 1.00 33.06 2963 O ALA B 725 43.630 8.759 102.838 1.00 36.69 2964 N GLY B 726 42.407 7.837 101.134 1.00 29.85 2965 CA GLY B 726 43.519 7.036 100.688 1.00 26.93 2966 C GLY B 726 44.531 8.080 100.151 1.00 31.48 2967 O GLY B 726 45.699 7.946 100.370 1.00 28.56 2968 N MET B 727 44.033 9.136 99.451 1.00 32.07 2969 CA MET B 727 44.899 10.121 98.846 1.00 32.07 2970 CB MET B 727 44.051 10.999 97.853 1.00 33.40 2971 CG MET B 727 45.180 9.612 95.806 1.00 35.66 2972 SD MET B 727 45.180 9.612 95.806 1.00 35.66 2973 CE MET B 727 46.441 10.934 95.492 1.00 31.92 2974 C MET B 727 46.441 10.934 95.492 1.00 31.10 2975 O MET B 727 46.780 11.331 99.892 1.00 31.10										
2963 O ALA B 725 43.630 8.759 102.838 1.00 36.69 2964 N GLY B 726 42.407 7.837 101.134 1.00 29.85 2965 CA GLY B 726 43.519 7.036 100.688 1.00 26.93 2966 C GLY B 726 44.531 8.080 100.151 1.00 31.48 2967 O GLY B 726 45.699 7.946 100.370 1.00 28.56 2968 N MET B 727 44.033 9.136 99.451 1.00 32.07 2969 CA MET B 727 44.091 10.121 98.846 1.00 33.27 2970 CB MET B 727 44.051 10.999 97.853 1.00 33.27 2971 CG MET B 727 45.180 9.612 95.806 1.00 31.54 2973 CE MET B 727 46.441 10.934 95.492 1.00 31.92 <										
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	2988					47.899				

FIGURE 3BH

A	В	С	D	E	F	G	Н	I	J
2989	CD1	TYR	В	729	48.409	6.323	105.122	1.00	31.09
2990	CE1	TYR		729	49.368		105.286	1.00	25.86
2991	CZ	TYR		729	49.864		104.160	1.00	32.58
2992	OH	TYR	В	729	50.764	3.772	104.302	1.00	30.28
2993	CE2	TYR	В	729	49.369	5.022	102.863	1.00	28.90
2994	CD2	TYR	В	729	48.343	5.918	102.735	1.00	28.62
2995	C	TYR	В	729	48.625	9.040	102.348	1.00	38.24
2996	0	TYR	В	729	49.760	9.011	102.837	1.00	40.23
2997	N	LEU	В	730	48.419	9.012	101.057		37.36
2998	CA	LEU	В	730	49.598	8.971	100.182		38.39
2999	CB	LEU	В	730	49.161	8.801	98.691		38.07
3000	CG	LEU	В	730	49.096	7.274	98.506		40.77
3001	CD1	LEU	В	730	48.033	6.879	97.535		46.74
3002		LEU		730	50.540	6.625	98.141		40.15
3003	C	LEU		730	50.415	10.239		1.00	36.79
3004	0	LEU		730	51.565	10.238			35.87
3005	N	ALA		731	49.753		100.211		38.07
3006	CA	ALA		731	50.421	12.597			41.33
3007	CB	ALA		731	49.377	13.802	100.342		35.88
3008	C	ALA		731	51.191		101.743		41.93
3009	0	ALA		731	52.353	12.861			41.92
3010	N	ASN		732	50.556	12.176			43.62
3011	CA	ASN		732	51.340	12.240			45.24
3012	CB	ASN		732	50.558 49.605	11.897 12.947			45.55 45.67
3013	CG OD1	ASN		732		14.047			45.78
3014 3015	OD1 ND2	ASN ASN		732 732	49.792 48.503	12.620			42.26
3015	C	ASN		732	52.439	11.247			46.19
3017	0	ASN		732	53.250		104.809		48.18
3018	N	MET		733	52.475	10.319			45.55
3019	CA	MET		733	53.611	9.396			42.71
3020	CB		В	733	53.181	8.051			43.29
3021	CG	MET		733	52.418	7.229			44.11
3022	SD	MET	В	733	53.390	6.662	104.809		45.37
3023	CE	MET		733	54.537	5.722	104.067	1.00	43.23
3024	C	MET	В	733	54.473	10.030	101.973	1.00	43.07
3025	0	MET	В	733	55.449	9.447	101.489	1.00	39.67
3026	N	ASN	В	734	54.114	11.288	101.639	1.00	45.47
3027	CA	ASN	В	734	54.895	11.978	100.620	1.00	45.76
3028	CB	ASN	В	734	56.293	12.036	101.146	1.00	48.02
3029	CG	ASN	В	734	56.917		100.855	1.00	55.08
,3030	OD1	ASN	В	734	57.998		100.227		57.65
3031	ND2	ASN	В	734	56.191		101.227		57.16
3032	C	ASN		734	55.017	11.329	99.233		44.84
3033	0	ASN		734	56.122	11.359	98.598		45.91
3034	N	TYR		735	53.933	10.733	98.723		43.14
3035	CA	TYR		735	53.846	10.348	97.298		39.99
3036	CB	TYR		735	53.511	8.904	97.196		42.06
3037	CG	TYR		735	54.612	7.939	97.303		39.82
3038	CD1			735	55.073	7.272			40.71
3039	CE1				56.143				49.17
3040	CZ	TYR	В	735	56.659	6.076	97.610	1.00	49.26

FIGURE 3BI

A	В	С	D	E	F	G	Н	I	J
3041	ОН	TYR	В	735	57.681	5.174	97.808	1.00	53.69
3042	CE2	TYR		735	56.180	6.710	98.706	1.00	46.44
3043	CD2	TYR		735	55.118	7.596	98.563		44.21
3044	C	TYR		735	52.766	11.131	96.513		40.01
3045	0	TYR		735	51.681	11.403	97.063		38.30
3046	N	VAL		736	53.084	11.534	95.242		39.05
3047	CA	VAL			52.155	12.135	94.317		37.57
3047	CB	VAL			52.978	12.826	93.220		40.62
3049	CG1	VAL			52.210	13.815	92.384	1.00	
3050	CG2	VAL		736	54.164	13.336	93.780		46.41
3051	C	VAL		736	51.824	10.887	93.435		37.17
	0	VAL		736	52.735	10.241	92.930		29.75
3052		HIS		737	50.539	10.241	93.185		37.35
3053	N			737	50.106	9.466	92.371		37.48
3054	CA	HIS		737	48.645	9.217	92.703		37.46
3055	CB	HIS				7.922	92.703		38.36
3056	CG	HIS		737	48.149 47.788		90.894		33.89
3057		HIS		737		7.709	90.753		38.45
3058	CE1	HIS		737	47.448	6.446	91.941		38.58
3059	NE2			737	47.527	5.845 6.737			36.23
3060	CD2			737	48.022		92.850		
3061	C	HIS		737	50.310	9.689	90.885		37.35 37.49
3062	0		В	737	50.900	8.930	90.179		
3063	N	ARG		738	49.921	10.862	90.420		41.12
3064	CA	ARG		738	50.156	11.215	89.025		41.82
3065	CB	ARG		738	51.548	10.752	88.576		42.45
3066	CG	ARG		738	52.900	11.362	89.171		43.81
3067	CD	ARG		738	53.934	12.099	88.306		50.41
3068	NE	ARG		738	54.475	11.640	87.014		59.49
3069	CZ	ARG		738	55.049	10.452	86.751		66.23
3070	NH1	ARG		738	55.115	9.499	87.671		66.49
3071	NH2	ARG		738	55.533	10.202	85.535		66.53
3072	C	ARG			49.061	10.581	88.104		42.10
3073	0	ARG		738	48.853	11.056	87.025		42.38
3074	N	ASP		739	48.304	9.578	88.572		40.65
3075	CA	ASP		739	47.402	8.839	87.683		37.25
3076	CB	ASP		739	48.098	7.585	87.132	1.00	
3077	CG	ASP	_		47.447	7.043	85.859		39.77
3078		ASP			46.714	7.845	85.259		35.07
3079		ASP			47.588	5.843	85.423		38.97
3080	C	ASP			46.159	8.470	88.383		33.96
3081	0	ASP			45.641	7.385	88.230		33.13
3082	N	LEU			45.612	9.440	89.054		32.76
3083	CA	LEU			44.385	9.304	89.792		32.28
3084	CB	LEU			44.218	10.378	90.903		28.90
3085	CG	LEU			42.918	10.273	91.633		31.41
3086		LEU			42.750	8.844	92.335		29.24
3087		LEU			42.714	11.301	92.751		31.09
3088	C	LEU			43.230	9.487	88.854		33.40
3089	0	LEU			42.972	10.631	88.367		32.41
3090	N	ALA			42.375	8.464	88.851		32.10
3091	CA	ALA			41.256	8.492	87.939		31.90
3092	CB .	ALA	В	741	41.795	8.228	86.473	1.00	25.99

FIGURE 3BJ

A	В	C	D	E	F	G	Н	I	J
3093	С	ALA		741	40.361	7.405	88.402		30.39
3094	0	ALA		741	40.849	6.468	89.090		32.43
3095	N	ALA		742	39.091	7.450	87.997		30.00
3096	CA	ALA		742	38.230	6.405	88.434		28.92
3097	CB	ALA		742	36.771	6.688	88.146		32.43
3098	C	ALA		742	38.702	5.046	87.904		31.77
3099	0	ALA		742	38.551	4.078	88.607		30.25
3100	N	ARG		743	39.282	4.907	86.696		31.71
3101	CA	ARG		743	39.685	3.568	86.348		32.57
3102	CB	ARG		743	40.311	3.530	84.893		30.75
3103	CG	ARG		743	41.249	4.519	84.625		29.61
3104	CD			743	42.260	4.076	83.465		43.52
3105	NE	ARG		743	43.297	5.113	83.400		45.54
3106	CZ	ARG		743	42.950	6.342	83.147		45.33
3107		ARG		743	41.651	6.558	82.868		38.16
3108		ARG		743	43.844	7.305	83.199		38.31
3109	C	ARG		743	40.697	3.045	87.291		32.35
3110	0	ARG		743	41.122	1.917	87.211		33.13
3111	N	ASN		744	41.306	3.909	88.055		33.51
3112	CA	ASN		744	42.357	3.337	88.857		32.87
3113	CB	ASN		744	43.651	4.144 3.813	88.701		33.36 34.78
3114	CG		В	744	44.393	2.792	87.400 86.820		48.21
3115				744 744	44.062		86.851		31.64
3116			В	744	45.248 41.888	4.718 3.251	90.300		34.12
3117 3118	C 0	ASN ASN		744	42.689	3.242	91.157		36.14
3119	N	ILE		745	40.592	3.314	90.558		32.33
3120	CA	ILE		745	40.098	3.112	91.861		31.92
3121	CB	ILE		745	39.154	4.230	92.239		31.00
3122	CG1	ILE		745	39.824	5.704	92.215		32.78
3123	CD1	ILE		745	41.204	5.701	92.993		32.89
3124	CG2		В	745	38.602	3.943	93.507		25.39
3125	С	ILE		745	39.347	1.767	91.809	1.00	32.48
3126	0	ILE		745	38.592	1.602	90.864	1.00	32.62
3127	N	LEU		746	39.593	0.833	92.752	1.00	29.93
3128	CA	LEU	В	746	38.994	-0.526	92.790	1.00	28.79
3129	CB	LEU	В	746	40.047	-1.578	93.158	1.00	27.96
3130	CG	LEU	В	746	41.188	-1.793	92.142	1.00	27.80
3131	CD1	LEU	В	746	42.431	-2.746	92.482		36.80
3132	CD2	LEU	В	746	40.582	-2.251	90.857		32.27
3133	C	LEU	В	746	37.941	-0.457	93.907		31.64
3134	0	LEU			38.176	0.242	94.933		32.71
3135	N	VAL			36.752	-1.061	93.727		32.95
3136	CA	VAL			35.729	-0.956	94.751		33.60
3137	CB	VAL			34.337	-0.627	94.211		35.06
3138		VAL			33.569	0.153	95.190		32.73
3139		VAL		747	34.311	-0.145	92.802		36.08
3140	C			747	35.379	-2.348	95.139		32.18
3141	0	VAL			35.438	-3.132	94.271		32.47
3142	N	ASN			34.809	-2.569	96.331		31.01
3143	CA			748	34.300	-3.873	96.670		32.11
3144	CB	ASN	R	748	35.076	-4.503	97.805	1.00	29.71

FIGURE 3BK

A	В	С	D	E	F	G	H	I	J
3145	CG	ASN	В	748	34.872	-3.789	99.093	1.00	30.19
3146		ASN		748	34.002	-2.965	99.154		29.21
3147		ASN		748	35.724		100.145		27.55
3148	С	ASN	В	748	32.782	-3.847	96.880	1.00	32.91
3149	0	ASN	В	748	32.137	-2.821	96.558	1.00	34.46
3150	N	SER	В	749	32.200	-4.931	97.392	1.00	31.86
3151	CA	SER	В	749	30.779	-4.924	97.589	1.00	32.16
3152	CB	SER	В	749	30.203	-6.341	97.762	1.00	33.15
3153	OG	SER	В	749	30.792	-7.147	98.772	1.00	33.73
3154	С	SER	В	749	30.390	-4.108	98.724	1.00	33.33
3155	0	SER	В	749	29.213	-3.877	98.965	1.00	31.39
3156	N	ASN	В	750	31.368	-3.666	99.517	1.00	34.87
3157	CA	ASN	В	750	30.972	-2.694	100.547		35.09
3158	CB	ASN	В	750	31.781		101.809		37.06
3159	CG	ASN		750	31.421		102.582		41.91
3160		ASN		750	30.278		102.549		38.82
3161		ASN		750	32.424		103.275		46.14
3162	C	ASN		750	31.082	-1.295	100.025		34.62
3163	0	ASN		750	30.760		100.737		36.26
3164	N	LEU		751	31.385	-1.151	98.738		31.97
3165	CA	LEU		751	31.511	0.150	98.134		33.21
3166	CB	LEU		751	30.275	1.085	98.379		33.30
3167	CG	LEU		751	28.944	0.583	97.933		29.08
3168		LEU		751	27.770	1.538	97.936		34.22
3169		LEU		751	29.187	0.432	96.569		25.04
3170	C	LEU		751	32.774	0.820	98.675		31.97
3171	O N	LEU		751	32.932	1.949	98.482 99.330		32.37 31.80
3172	N	VAL VAL		752 752	33.673 34.884	0.112 0.756	99.838		32.23
3173 3174	CA CB	VAL			35.557		100.847		34.25
3174		VAL		752	36.916	0.159			28.08
3175	CG2	VAL		752	34.701		102.072		27.86
3177	C	VAL		752	35.761	0.974	98.604		34.48
3178	Ö	VAL		752	35.900	0.035	97.753		33.89
3179	N	CYS		753	36.345	2.183	98.450		34.53
3180	CA	CYS		753	37.139	2.463	97.238		33.46
3181	CB	CYS		753	36.667	3.795	96.590		32.57
3182	SG	CYS			35.024	3.589	95.866		33.85
3183	C	CYS			38.595	2.504	97.641		32.87
3184	0	CYS	В	753	38.918	2.994	98.661	1.00	33.65
3185	N			754	39.490	2.019		1.00	31.25
3186	CA			754	40.879	2.069	97.142	1.00	28.59
3187	CB	LYS	В	754	41.393	0.682	97.601	1.00	28.62
3188	CG	LYS	В	754	40.612	0.009	98.777	1.00	25.26
3189	CD	LYS	В	754	41.255	-1.359	99.092	1.00	26.47
3190	·CE	LYS	В	754	40.451		100.084	1.00	31.42
3191	NZ	LYS	В	754	41.028		101.467		36.53
3192	C	LYS	В	754	41.659	2.488	95.931		29.63
3193	0	LYS			41.451	1.951	94.764		29.44
3194	N	VAL			42.643	3.336			28.68
3195	CA	VAL			43.512	3.819			30.76
3196	CB	VAL	В	755	44.484	4.852	95.681	1.00	29.87

FIGURE 3BL

Α .	В	С	D	E	F	G	Н	I	J
3197	CG1	VAL	В	755	45.380	5.460	94.520	1.00	26.20
3198		VAL			43.750	5.907	96.257		28.72
3199	C	VAL			44.391	2.708	94.759		31.83
3200	0	VAL			44.894	2.059	95.618		30.86
3201	N			756	44.722	2.641	93.486		33.08
3202	CA	SER			45.431	1.545	92.914		36.43
3202	CB	SER			44.472	0.481	92.259		37.70
3204	OG	SER			45.281	-0.617	91.571		40.69
3205	C	SER			46.368	2.061	91.849		37.72
3205	0	SER			46.466	3.263	91.576		37.99
3207	N	ASP			46.978	1.130	91.147		38.48
3208	CA	ASP			47.861	1.499	90.074		41.72
3209	CB	ASP			47.023	1.917	88.888		41.39
3210	CG	ASP			47.849	1.913	87.574		50.91
3211		ASP			47.211	2.091	86.487		51.60
3212		ASP		757	49.141	1.757	87.558		52.69
3212	C	ASP		757	49.001	2.490	90.467		41.65
3214	0	ASP		757	48.943	3.671	90.267		41.11
3215	N	PHE		758	50.076	1.995	91.048		43.52
3215	CA	PHE			51.087	2.948	91.493		44.14
3217	CB	PHE			51.525	2.631	92.952		43.50
3217	CG	PHE			50.456	2.888	93.920		38.35
3219		PHE			50.308	4.177	94.499		33.03
3220	CE1	PHE			49.233	4.488	95.392		33.75
3221	CZ	PHE		758	48.282	3.458	95.734		35.68
3222		PHE		758	48.419	2.141	95.050		35.33
3223		PHE			49.531	1.901	94.184		37.29
3224	C	PHE			52.199	3.247	90.454		45.65
3225	0	PHE			53.160	4.088	90.646		46.52
3226	N	GLY			51.903	2.709	89.282		46.03
3227	CA	GLY		759	52.617	2.856	88.048		47.12
3228	C	GLY		759	53.353	4.173	87.857		50.02
3229	0	GLY		759	54.588	4.163	87.553		53.05
3230	N	LEU		760	52.664	5.294	87.911		46.21
3231	CA	LEU		760	53.371	6.532	87.683		47.41
3232	CB	LEU		760	52.504	7.502	86.833		46.97
3233	CG	LEU	В	760	52.025	7.054	85.450		52.65
3234		LEU	В	760	51.187	8.062			51.82
3235		LEU			53.252				51.03
3236	С	LEU	В	760	53.628	7.284	88.974	1.00	47.35
3237	0	LEU			53.755		88.928	1.00	47.23
3238	N	SER			53.643		•		48.54
3239	CA	SER			53.583	7.610	91.262		49.64
3240	CB	SER			52.674	7.066	92.329	1.00	47.14
3241	OG	SER			53.142	5.812	92.428		48.99
3242	С	SER			54.965	7.803	91.813	1.00	50.77
3243	0	SER			55.814	6.895	91.672		51.89
3244	N	ARG			55.227	8.947	92.427		50.64
3245	CA	ARG			56.576	9.132	92.940	1.00	51.02
3246	CB	ARG				9.689	91.897	1.00	52.96
3247	CG	ARG			57.051			1.00	55.70
3248	CD	ARG			57.559			1.00	67.92

FIGURE 3BM

A	В	С	D	E	F	G	Н	I	J
3249	NE	ARG	В	762	57.115	8.769	88.974	1.00	75.81
3250	CZ	ARG		762	57.530	8.088	87.860	1.00	79.84
3251	NH1			762	57.034	6.858	87.589	1.00	77.74
3252	NH2	ARG		762	58.432	8.624	87.030	1.00	79.01
3253	С	ARG	В	762	56.692	9.874	94.202	1.00	50.69
3254	0	ARG	В	762	55.762	10.587	94.600	1.00	50.50
3255	N	VAL	В	763	57.834	9.667	94.879	1.00	52.25
3256	CA	VAL	В	763	58.143	10.438	96.111	1.00	53.91
3257	CB	VAL	В	763	59.438	9.932	96.770	1.00	56.45
3258	CG1	VAL	В	763	59.822	10.769	98.058	1.00	53.41
3259	CG2	VAL	В	763	59.293	8.431	97.046	1.00	53.98
3260	C	VAL	В	763	58.323	11.921	95.757	1.00	52.61
3261	0	VAL	В	763	58.998	12.205	94.849	1.00	52.54
3262	N	ALA	В	764	57.680	12.818	96.460	1.00	53.25
3263	CA	ALA		764	57.640	14.215	96.083	1.00	55.20
3264	CB	ALA	В	764	56.842	15.013	97.079	1.00	55.95
3265	С	ALA	В	764	58.997	14.901	95.822	1.00	58.47
3266	0	ALA	В	764	60.011	14.667	96.486	1.00	58.95
3267	N	ALA		778	52.512	8.707	77.650	1.00	63.16
3268	CA	ALA		778	53.274	9.379	78.726	1.00	64.24
3269	CB	ALA		778	54.203	10.520	78.164	1.00	63.79
3270	C	ALA		778	52.320	9.882	79.851	1.00	63.12
3271	0	ALA		778	52.320	9.355	80.966	1.00	63.11
3272	N	ILE		779	51.472	10.863	79.572	1.00	61.82
3273	CA			779	50.565	11.342	80.639	1.00	59.71
3274	CB			779	51.075	12.717	81.033	1.00	60.71
3275	CG1	ILE		779	52.166	12.503	82.090	1.00	62.19
3276	CD1	ILE		779	53.432	13.193	81.727	1.00	66.21
3277	CG2	ILE		779	49.943	13.685	81.434	1.00	62.88
3278	C	ILE		779	49.010	11.248	80.435	1.00	57.07
3279	0	ILE	В	779	48.552	11.065	79.280	1.00	55.98
3280	N			780	48.228	11.201	81.549	1.00	54.65 52.75
3281	CA	PRO		780	46.770	11.559 11.448	81.509 82.969	1.00	53.47
3282	CB	PRO PRO		780	46.321 47.247	11.448 10.442	83.543	1.00	51.28
3283	CG CD			780 780	48.603	10.442	82.915	1.00	54.55
3284 3285	CD	PRO		780	46.610	12.952	81.191		50.88
3286	0	PRO		780	46.988	13.770	82.008		56.60
3287	N	ILE		781	46.112	13.770	80.017		46.48
3288	CA	ILE		781	45.849	14.560	79.767		43.01
3289	CB	ILE		781	45.897	14.790	78.286		41.97
3290	CG1	ILE		781	47.316	15.269	78.013		45.31
3291	CD1	ILE		781	48.308	14.194	77.831		50.28
3292	CG2	ILE		781	45.107	15.941	77.979		38.03
3293	C	ILE		781	44.611	15.023	80.581		40.95
3294	Ō	ILE		781	44.748	15.814	81.489		40.34
3295	N	ARG		782	43.460	14.431	80.284		41.60
3296	CA	ARG		782	42.166	14.646	80.837		38.55
3297	CB	ARG		782	41.127	13.968	79.858		40.91
3298	CG	ARG		782	40.395	12.734	80.126		39.72
3299	CD	ARG		782	40.142	12.040	78.779		44.03
3300	NE			782	38.977	12.556	78.126	1.00	50.70

FIGURE 3BN

A	В	С	D	E	F	G	Н	I	J
	a =	200	_	700	28 676	12 000	76 050	1 00	F0 20
3301	CZ	ARG			38.978	13.000	76.853		52.30
3302	NH1	ARG		782	37.828	13.451	76.324		46.70
3303		ARG		782	40.126	13.022	76.153	1.00	
3304	C	ARG		782	42.033	14.486	82.369	1.00	
3305	0	ARG		782	41.124	15.127	82.932	1.00	
3306	N	TRP		783	42.986	13.873	83.062	1.00	
3307	CA	TRP		783	42.931	13.863	84.548		36.23
3308	CB	TRP		783	43.045	12.446	85.168		35.36
3309	CG	TRP		783	41.939	11.580	84.894		34.89
3310	CD1	TRP		783	40.959	11.347	85.728		34.55
3311	NE1	TRP		783	40.032	10.518	85.152		35.15
3312	CE2	TRP		783	40.417	10.196	83.889	1.00	
3313	CD2	TRP	В	783	41.611	10.885	83.662	1.00	
3314	CE3	TRP	В	783	42.243	10.720	82.424	1.00	
3315	CZ3	TRP	В	783	41.642	9.873	81.461	1.00	
3316	CH2	TRP		783	40.386	9.270	81.697		30.32
3317	CZ2	TRP	В	783	39.750	9.394	82.892		26.79
3318	C	TRP	В	783	44.019	14.767	85.182	1.00	37.26
3319	0	TRP	В	783	44.078	14.934	86.462	1.00	32.75
3320	N	THR	В	784	44.868	15.335	84.294	1.00	38.13
3321	CA	THR	В	784	46.074	16.069	84.782	1.00	38.14
3322	CB	THR	В	784	47.220	15.822	83.921	1.00	38.22
3323	OG1	$\cdot \text{THR}$	В	784	47.407	14.394	83.791	1.00	32.84
3324	CG2	THR	В	784	48.499	16.365	84.574	1.00	27.62
3325	C	THR	В	784	45.959	17.558	84.819	1.00	42.12
3326	0	THR	В	784	45.451	18.183	83.855	1.00	44.07
3327	N	ALA	В	785	46.415	18.118	85.944	1.00	42.78
3328	CA	ALA	В	785	46.490	19.525	86.209	1.00	42.20
3329	CB	ALA	В	785	47.126	19.714	87.503	1.00	41.73
3330	C	ALA	В	785	47.330	20.250	85.152	1.00	42.59
3331	0	ALA	В	785	48.358	19.707	84.633	1.00	41.88
3332	N	PRO	В	786	46.867	21.443	84.823	1.00	41.88
3333	CA	PRO	В	786	47.509	22.281	83.783	1.00	43.28
3334	CB	PRO	В	786	46.514	23.437	83.610	1.00	42.82
3335	CG	PRO	В	786	45.682	23.472	84.854	1.00	38.60
3336	CD	PRO	В	786	45.625	22.022	85.316	1.00	40.34
3337	C	PRO	В	786	48.937	22.647	84.199	1.00	44.36
3338	0	PRO	В	786	49.876	22.335	83.415	1.00	43.75
3339	N	GLU	В	787	49.161	23.067	85.458	1.00	47.66
3340	CA	GLU	В	787	50.585	23.216	85.879	1.00	48.56
3341	CB	GLU	В	787	50.799	23.521	87.366	1.00	50.25
3342	CG	GLU	В	787	50.506	22.415	88.438	1.00	47.77
3343	CD	GLU	В	787	49.055	22.343	88.835	1.00	45.14
3344	OE1	GLU	В	787	48.239	23.053	88.217	1.00	47.89
3345	OE2	GLU	В	787	48.675	21.581	89.750	1.00	48.40
3346	C	GLU	В	787	51.413	22.011	85.524	1.00	48.85
3347	0	GLU	В	787	52.601	22.103	85.448	1.00	49.02
3348	N	ALA			50.810	20.871	85.240	1.00	50.59
3349	CA	ALA			51.630	19.703	85.119	1.00	52.43
3350	CB	ALA			51.138	18.650	85.984	1.00	53.63
3351	C	ALA			51.881		83.771		54.39
3352	0	ALA			52.825	18.429			53.44

FIGURE 3BO

A	В	С	D	E		F		G		Н	I	J
3353	N·	ILE	В	789	51	L.076	19.	.709	82	.848	1.00	58.49
3354	CA	ILE		789	51	1.180	19.	. 309	81	.466	1.00	60.06
3355	СВ	ILE		789		791	19.	422	80	.879	1.00	60.19
3356	CG1		В	789	49	0.005	18.	.288	81	.542	1.00	57.40
3357	CD1	ILE		789		7.545		.338	81	.498	1.00	52.54
3358	CG2	ILE		789		888.		. 223	79	.405		60.76
3359	C	ILE		789		2.175		.260		.860		61.11
3360	0	ILE		789		3.217		.903		.277	1.00	61.28
3361	N	SER		790		L.775		.498		.090	1.00	63.37
3362	CA	SER		790		2.455		.746		.870		65.13
3363	СВ	SER		790		L.887	23.	. 687	81	.908	1.00	64.75
3364	OG	SER		790		2.132	22.	. 945	83	.109	1.00	72.95
3365	C	SER		790		3.883		.498		.324	1.00	65.49
3366	0	SER		790		1.721		.181		.519	1.00	65.88
3367	N	TYR		791	54	1.080		.534	82	.650	1.00	67.60
3368	CA	TYR		791		5.356		. 655	83	.371	1.00	67.61
3369	CB	TYR		791		5.133		. 658	84	.492	1.00	67.72
3370	CG	TYR		791		1.527		.979	84	.072	1.00	69.06
3371	CD1	TYR		791		3.373		.468	84	.681	1.00	73.54
3372	CE1	TYR		791		2.811	26	.729	84	.343	1.00	77.27
3373	CZ	TYR		791		3.434	27.	.536	83	.361	1.00	78.11
3374	OH	TYR		791		2.888		.779		.031	1.00	74.15
3375	CE2	TYR		79 1	54	1.617	27	.080	82	.777	1.00	76.67
3376	CD2	TYR		791		5.167	25	.794	83	.142	1.00	74.63
3377	C	TYR		791	55	5.841	21	.341	83	.987	1.00	67.44
3378	0	TYR		791	56	5.991	21	.177	84	.471	1.00	66.78
3379	N	ARG	В	792	54	1.955	20	.377	83	.993	1.00	66.21
3380	CA	ARG	В	792	55	5.418	19	.098	84	.530	1.00	65.39
3381	CB	ARG	В	792	56	5.655	18	.642	83	.811	1.00	65.99
3382	CG	ARG	В	792	56	5.702	17	.131	83	.750	1.00	72.90
3383	CD	ARG	В	792	57	7.978	16	.532	83	.158	1.00	81.61
3384	NE	ARG	В	792	58	3.984	17	.572	83	.010	1.00	88.48
3385	CZ	ARG	В	792	60	0.191	17	.394	82	.478		91.91
3386	NH1	ARG	В	792	60	0.980	18	.468	82	.408	1.00	92.54
3387	NH2	ARG	В	792	60	0.592	16	.196	82	.009		89.53
3388	C	ARG	В	792		5.624	19	.127		.033	1.00	61.73
3389	0	ARG		792		5.452		.430		.557		61.41
3390	N	ALA	В	793	54	1.792		.903		.722		58.85
3391	CA			793		1.853				.179		56.36
3392	CB	ALA	В	793	54	1.957		.543		.590		55.91
3393	C	ALA	В	793		3.713		.275		.952		55.37
3394	0			793		2.576		.774		.157		53.05
3395	N			794		1.087		.085		.403		53.01
3396	CA			794		3.197		.141		.066		52.23
3397	CB			794		3.621		.682		.718		51.93
3398	CG	PHE		794		3.400		.338		.275		52.20
3399		PHE		794		2.102		. 265		.761		55.84
3400		PHE				L.857		.993		.368		57.33
3401	CZ	PHE		794		2.972		.849		.527		57.10
3402		PHE				1.271				.076		51.98
3403		PHE				1.461				.425		50.42
3404	C	PHE	В	794	53	3.311	17	.374	91	.542	1.00	50.46

FIGURE 3BP

A	В	C	D	E	F	G	Н	I	J
3405	0			794	54.347	17.425	92.050		51.33
3406	N	THR		795	52.221	17.321	92.249		49.78
3407	CA	THR		795	52.232	17.820	93.561		47.81
3408	CB	THR		795	52.007	19.294	93.227	1.00	
3409	OG1	THR		795	53.044	20.092	93.792		53.29
3410	CG2	THR		795	50.667	19.849	93.729		46.81
3411	C	THR		795	50.983	17.224	94.222		46.44
3412	0	THR		795	50.005	16.921	93.564		45.65
3413	N	SER		796	50.946	17.050	95.504		42.66
3414	CA	SER		796	49.646	16.708	95.943		42.64
3415	CB	SER	В	796	49.536	16.690	97.500		42.15
3416	OG	SER		796	50.321	15.565	97.792		41.91
3417	C	SER	В	796	48.526	17.544	95.328		41.72
3418	0	SER	В	796	47.377	17.048	95.157		41.30
3419	N	ALA	В	797	48.784	18.819	95.079		40.89
3420	CA	ALA	В	797	47.663	19.681	94.615		40.50
3421	CB	ALA	В	797	48.022	21.114	94.671		39.74
3422	C	ALA		797	47.280	19.305	93.173		39.17
3423	0	ALA	В	797	46.128	19.595	92.751		38.84
3424	N	SER	В	798	48.263	18.720	92.489	1.00	
3425	CA	SER	В	798	48.225	18.096	91.130	1.00	37.20
3426	CB	SER	В	798	49.628	17.544	91.024	1.00	36.03
3427	OG	SER	В	798	50.147	17.397	89.784	1.00	39.62
3428	C	SER	В	798	47.230	16.905	91.257	1.00	37.26
3429	0	SER	В	798	46.155	16.860	90.659		39.61
3430	N	ASP	В	799	47.482	16.037	92.210	1.00	38.19
3431	CA	ASP	В	799	46.573	14.920	92.473	1.00	37.01
3432	CB	ASP	В	799	47.107	14.077	93.579	1.00	35.52
3433	CG	ASP	В	799	48.139	13.180	93.147		34.06
3434			В	799	48.373	13.014	91.930	1.00	35.46
3435	OD2	ASP	В	799	48.888	12.613	93.969		38.80
3436	C	ASP	В	799	45.199	15.458	92.855		35.89
3437	0		В	799	44.175	14.779	92.609		37.05
3438	N			800	45.142	16.620	93.477		35.26
3439	CA			800	43.822	17.145	93.947	1.00	32.94
3440	CB	VAL			43.940	18.266	95.019	1.00	
3441		VAL			42.646	19.149	95.117		22.48
3442	CG2	VAL	В	800	44.469	17.699	96.515		28.48
3443	C	VAL			42.950		92.768		34.34
3444	0	VAL			41.709				35.47
3445	N			801	43.636				34.34
3446	CA	TRP	В	801	43.044	18.275			35.48
3447	CB				44.091	18.901	89.507		35.00
3448	CG	TRP	В	801	43.459	19.177	88.157		40.40
3449	CD1				43.141	18.226	87.174		38.90
3450		TRP			42.553	18.884			39.62
3451	CE2			801	42.424				34.39
3452		TRP			43.007				34.20
3453	CE3	TRP	В	801	43.005				38.91
3454	C Z 3	TRP	В	801	42.445		87.399		36.57
3455	CH2	TRP	В	801	41.952	22.492			36.98
3456	CZ2	TRP	В	801	41.885	21.221	85.652	1.00	38.72

FIGURE 3BQ

3457 C TRP B 801 42.351 16.959 89.962 1.00 3	33.13
3458 O TRP B 801 41.094 16.871 89.763 1.00 3	32.82
3459 N SER B 802 43.167 15.932 89.804 1.00 3	
3460 CA SER B 802 42.670 14.644 89.377 1.00 3	30.99
3461 CB SER B 802 43.764 13.696 89.596 1.00 3	32.92
3462 OG SER B 802 44.915 13.966 88.873 1.00 2	
3463 C SER B 802 41.511 14.199 90.191 1.00 3	
	33.27
3465 N PHE B 803 41.612 14.494 91.467 1.00 3	
3466 CA PHE B 803 40.592 14.026 92.333 1.00 2	
3467 CB PHE B 803 40.976 14.324 93.828 1.00 2	
3468 CG PHE B 803 39.873 14.000 94.769 1.00 2	
3469 CD1 PHE B 803 39.025 15.007 95.261 1.00 2	
3470 CE1 PHE B 803 38.016 14.683 96.177 1.00 3	
3471 CZ PHE B 803 37.764 13.282 96.514 1.00 3	
3472 CE2 PHE B 803 38.619 12.258 95.929 1.00 2	
3473 CD2 PHE B 803 39.656 12.633 95.129 1.00 3	
3474 C PHE B 803 39.283 14.713 92.014 1.00 2	
3475 O PHE B 803 38.185 14.221 92.288 1.00 2	
3476 N GLY B 804 39.385 15.925 91.508 1.00 3	
3477 CA GLY B 804 38.192 16.682 91.178 1.00 3	
3478 C GLY B 804 37.595 15.997 89.930 1.00 3	
3479 O GLY B 804 36.344 15.792 89.811 1.00 3	
3480 N ILE B 805 38.471 15.468 89.086 1.00 3	
3481 CA ILE B 805 37.922 14.809 87.937 1.00 3	
3482 CB ILE B 805 39.019 14.336 86.958 1.00 3	
3483 CG1 ILE B 805 39.901 15.503 86.501 1.00 2	
3484 CD1 ILE B 805 39.060 16.699 85.638 1.00 2	
3485 CG2 ILE B 805 38.273 13.590 85.789 1.00 3	
3486 C ILE B 805 37.187 13.531 88.399 1.00 3	
	30.88
3488 N VAL B 806 37.856 12.771 89.253 1.00 3	
3489 CA VAL B 806 37.335 11.519 89.853 1.00 2	
3490 CB VAL B 806 38.295 10.897 90.978 1.00 2	
3491 CG1 VAL B 806 37.674 9.730 91.601 1.00 2	
3492 CG2 VAL B 806 39.518 10.536 90.425 1.00 2	
3493 C VAL B 806 36.055 11.924 90.505 1.00 2	
3494 O VAL B 806 35.066 11.258 90.312 1.00 3	
3495 N MET B 807 36.006 12.981 91.282 1.00 2	
3496 CA MET B 807 34.635 13.320 91.782 1.00 3	
3497 CB MET B 807 34.544 14.686 92.556 1.00 2	
3498 CG MET B 807 35.490 14.830 93.746 1.00 2	
3499 SD MET B 807 35.350 16.540 94.517 1.00 3	
3500 CE MET B 807 33.929 16.536 95.089 1.00 3	
3501 C MET B 807 33.615 13.403 90.606 1.00 3	
3502 O MET B 807 32.442 13.037 90.717 1.00 3	
3503 N TRP B 808 34.040 13.980 89.473 1.00 3	
3504 CA TRP B 808 33.026 14.215 88.453 1.00 2	
3505 CB TRP B 808 33.626 15.123 87.374 1.00 3	
3506 CG TRP B 808 32.681 15.593 86.292 1.00 2	
3507 CD1 TRP B 808 31.826 16.670 86.368 1.00 2	
3508 NE1 TRP B 808 31.178 16.794 85.186 1.00 3	

FIGURE 3BR

A	В	C	D	E	F	G	Н	I	J
3509	CE2	TRP	В	808	31.566	15.779	84.355	1.00	32.11
3510	CD2	TRP			32.468	14.980	85.061		28.97
3511	CE3	TRP		808	33.064	13.909	84.398		28.52
3512	CZ3			808	32.709	13.687	83.032	1.00	32.24
3513	CH2	TRP		808	31.725	14.446	82.425	1.00	
3514	CZ2	TRP			31.185	15.521	83.050	1.00	
3515	C	TRP		808	32.712	12.873	87.869	1.00	28.00
3516	0			808	31.577	12.568	87.668	1.00	31.29
3517	N			809	33.684	12.013	87.650		27.30
3518	CA	GLU	В	809	33.330	10.714	87.110	1.00	28.51
3519	CB	GLU	В	809	34.555	9.884	86.910	1.00	30.85
3520	CG	GLU	В	809	35.617	10.432	86.024	1.00	25.12
3521	CD	GLU	В	809	36.813	9.571	86.014	1.00	28.19
3522	OE1	GLU	В	809	36.849	8.704	85.133	1.00	32.40
3523	OE2	GLU	В	809	37.778	9.798	86.791	1.00	31.60
3524	С	GLU	В	809	32.435	9.919	88.019	1.00	30.07
3525	0	GLU	В	809	31.575	9.111	87.555	1.00	33.66
3526	N	VAL	В	810	32.507	10.201	89.289	1.00	30.06
3527	CA	VAL	В	810	31.716	9.434	90.205	1.00	29.76
3528	CB	VAL	В	810	32.255	9.428	91.665	1.00	30.24
3529	CG1	VAL	В	810	31.095	9.097	92.609	1.00	24.88
3530	CG2	VAL	В	810	33.391	8.481	91.834	1.00	25.13
3531	C	VAL	В	810	30.346	10.058	90.287	1.00	30.62
3532	0	VAL	В	810	29.381	9.349	90.313	1.00	27.09
3533	N	MET	В	811	30.247	11.393	90.308	1.00	32.39
3534	CA	MET	В	811	28.889	11.928	90.411		34.71
3535	CB	MET	В	811	28.900	13.402	90.899		35.87
3536	CG	MET			29.590	13.624	92.224		38.06
3537	SD	MET			28.965	12.583	93.435		43.12
3538	CE	MET			27.111	12.868	93.575		35.71
3539	C	MET			28.162	11.746	89.043		33.74
3540	0	MET			27.022	11.928	88.905		36.24
3541	N			812	28.845	11.231	88.066		35.66
3542	CA			812	28.304	11.132	86.752		35.64
3543	CB	THR		812	29.319	11.867	85.953		37.45
3544	OG1	THR		812	28.697	12.834	85.169	1.00	
3545	CG2				30.251	11.113	85.174		23.27
3546		THR			28.173	9.753	86.352		37.54 38.76
3547	0			812	27.786 28.448		85.230		
3548	N			813					37.57 34.78
3549	CA			813	28.363				34.82
3550	CB			813	26.962		86.721 88.076		34.63
3551	CG CD1			813	26.132 25.269	6.832 7.812	88.444		29.08
3552	CD1	TYR				7.762	89.559		29.89
3553 3554	CE1 CZ	TYR		813	24.637 24.749	6.694	90.445		35.16
	OH			813	23.994	6.732	91.691		33.13
3555 3556	CE2	TYR			25.605	5.638	90.112		31.34
3557	CD2	TYR			26.330	5.766			30.20
3557 3558	C			813	29.301	6.978			34.15
3559	0			813	28.981		85.162		35.41
3560	N			814	30.513	7.539			33.63
5500	**		ب	V	30.313				00

FIGURE 3BS

A	В	C	D	E	F	G	Н	I	J
3561	CA			814	31.485	6.912	85.013		33.04
3562	C			814	31.465	7.503	83.656		33.66
3563	0			814	31.929	6.919	82.671		29.15
3564	N			815	30.913	8.688	83.576		34.73
3565	CA			815	31.053	9.319	82.301		37.09
3566	CB			815	30.177	10.491	82.237		38.02
3567	CG			815	30.303	11.378	80.999		40.70
3568	CD			815	29.679	10.720	79.825		39.58
3569		GLU			30.404	10.091	79.087		37.45
3570		GLU			28.456	10.675	79.743		43.36
3571	C			815	32.498	9.735	82.095		38.19
3572	0			815	33.212	10.124	83.020		38.65
3573	N			816	32.930	9.543	80.863		37.01
3574	CA			816	34.213	9.930	80.391		38.78
3575	CB			816	34.352	9.446	78.966		38.98
3576	CG			816	35.424	10.059	78.162		42.28
3577	CD			816	36.087	9.017	77.341		
3578	NE			816	37.532	9.132 9.580	77.360		54.71 59.21
3579	CZ	ARG		816	38.138	9.500	76.306 75.305	1.00	
3580					37.353	9.779	76.226	1.00	
3581 3582		ARG			39.446	11.410	80.467		38.72
	С О			816 816	34.381 33.687	12.139	79.791		39.78
3583 3584				817	35.330	11.824	81.298		37.40
3585	N CA			817	35.684	13.217	81.461		37.95
3586	CB			817	36.997	13.136	82.256		37.05
3587	CG			817	36.763	11.888	83.183		38.15
3588	CD			817	36.171	10.927	82.136		38.41
3589	C			817	35.788	13.947	80.089		38.69
3590	ō			817	36.495	13.433	79.252		36.60
3591	N			818	35.057	15.066	79.844		38.82
3592	CA			818	35.210	15.759	78.539		39.23
3593	CB			818	36.663	16.068	78.236		38.09
3594	CG			818	37.266	16.821	79.315		39.70
3595	CD1	TYR			36.909	18.157	79.532		34.79
3596	CE1	TYR			37.443	18.905	80.645		34.86
3597	CZ			818	38.325	18.209	81.532	1.00	37.76
3598	OH			818	38.860			1.00	39.95
3599	CE2	TYR	В	818	38.653	16.824	81.335	1.00	33.51
3600	CD2				38.098	16.158	80.229	1.00	36.26
3601	C			818	34.667	14.938	77.424	1.00	38.80
3602	0			818	34.928	15.202	76.270	1.00	39.89
3603	N	TRP	В	819	33.846	13.989	77.763	1.00	38.70
3604	CA	TRP	В	819	33.188	13.270	76.700	1.00	39.85
3605	CB	TRP	В	819	32.069	14.135	76.151	1.00	38.03
3606	CG	TRP			31.456	14.694	77.287	1.00	36.05
3607	CD1				30.606	14.112	78.042	1.00	30.08
3608	NE1	TRP			30.225	14.945	79.039	1.00	25.80
3609	CE2	TRP			30.803	16.169	78.851	1.00	30.10
3610	CD2	TRP			31.604	16.053	77.781	1.00	36.77
3611	CE3	TRP			32.310	17.173	77.346	1.00	33.18
3612	CZ3	TRP	В	819	32.236	18.266	77.979	1.00	31.31

FIGURE 3BT

A	В	C	D	E	F	?	G		Н	I	J
3613	CH2	TRP	В	819	31.4	110 18	3.424	79	.081	1.00	35.76
3614	CZ2	TRP			30.6		7.374		.552		36.26
3615	C	TRP			34.1		2.981		.636		39.50
3616	Ō			819	35.2		2.601		.950		42.24
3617	N	GLU			33.8		3.251		.389		39.99
3618	CA	GLU			34.7		2.918		. 254		40.61
3619	СВ	GLU		820	33.9		2.178		.114	1.00	41.25
3620	CG	GLU	В	820	33.2	263 10	0.859	72	.529	1.00	40.27
3621	CD	GLU	В	820	32.0	030 13	L.030	73	.446	1.00	45.99
3622	OE1	GLU	В	820	31.8	375 10	.407	74	.529	1.00	48.82
3623	QE2	GLU	В	820	31.1	163 13	L.766	7 3	.086	1.00	36.20
3624	C	GLU	В	820	35.7	708 14	1.020	72	.749	1.00	40.02
3625	0	GLU	В	820	36.2	216 13	3.972	71	.706	1.00	39.30
3626	N	LEU	В	821	35.9		5.037	73	.516	1.00	42.32
3627	CA	LEU	В	821	36.9	969 16	5.002	73	.125	1.00	45.66
3628	CB	LEU	В	821	37.2	212 16	5.973	74	.283	1.00	45.63
3629	CG	LEU			36.2		3.189		.253		50.25
3630	CD1				34.8		7.908		.740		53.81
3631		LEU			36.2		3.988		.530		46.51
3632	C	LEU		821	38.2		5.199		.892		45.45
3633	0	LEU			38.3		1.137		.411		45.58
3634	N	SER			39.1		5.665		.097		45.03
3635	CA	SER			40.4		1.994		.975		47.64
	CB	SER			41.2		5.426		.738		47.83
3637	OG	SER			41.4		5.836		.727		44.19
3638	C	SER			41.2		5.448		.115		48.61
3639	0	SER			40.9		5.431		.769		48.62
3640	N	ASN			42.4		1.776		.341		50.08
3641	CA	ASN			43.3		3.385		.319	1.00	53.14 53.45
3642	CB	ASN			44.4		1.436		.614	1.00	57.25
3643	CG	ASN			43.9		3.177 3.236				56.44
3644		ASN ASN			42.9 44.6		2.035		.090 .027		50.82
3645 3646	C C	ASN			43.6		5.895		.027		52.98
3647	0	ASN			43.3		7.756		.937		53.13
3648	N	HIS			44.1		7.237		.858		54.65
3649	CA	HIS			44.4		3.636		.459		54.79
3650		HIS					3.740		.973		58.59
3651	CG	HIS			44.1		9.419		.940		67.70
3652		HIS			43.6		0.705		.072		73.79
3653		HIS			42.8		L.017		.000		75.94
3654		HIS			42.7		0.940		.073		75.8 7
3655		HIS			42.9		9.999		.157		76.47
3656		HIS			43.7		3.994		.703	1.00	75.66
3657	С	HIS			43.3		9.509	72	.778	1.00	52.56
3658	0	HIS			43.4		588	73	.463	1.00	49.91
3659	N	GLU			42.3		9.027		.387	1.00	50.66
3660	CA	GLU			40.9	942 19	9.831	72	.718	1.00	50.31
3661	CB	GLU	В	825	39.6	599 19	9.255	72	.086	1.00	52.70
3662	CG	GLU	В	825	39.9	956 18	3.712		.695		55.19
3663	CD	GLU	В	825	38.7	704 18	3.188		.065		60.55
3664	OE1	GLU	В	825	38.4	180 16	5.987	70	.221	1.00	63.97

FIGURE 3BU

3665 OB2 GLU B 825	A	В	С	D	E	F	G	Н	I	J
3666 C GLU B 825 40.747 20.079 74.206 1.00 49.70 3667 O GLU B 825 40.538 21.250 74.669 1.00 47.68 3668 N VAL B 826 40.903 19.012 74.976 1.00 47.64 3670 CB VAL B 826 40.932 19.160 76.439 1.00 46.21 3671 CGI VAL B 826 41.173 17.756 77.124 1.00 46.21 3672 CGZ VAL B 826 40.130 16.592 76.663 1.00 46.74 3673 C VAL B 826 41.762 20.239 76.581 1.00 46.67 3674 O VAL B 826 41.363 12.236 77.651 1.00 46.61 3675 C MET B 827 44.025 21.031 77.016 1.00 46.61 3677 CB MET B 827 44.025 21.031 77.106 1.00 44.63 3679 SD MET B 827 46.402 1.007 76.541 1.00 49.16	3665	OE2	GLU	В	825	37.946	18.964	69.435	1.00	63.96
3667 O GLU B 825										
3668 N VAL B 826 40.903 19.012 74.976 1.00 47.68 3669 CA VAL B 826 40.825 19.160 76.439 1.00 46.21 3670 CB VAL B 826 41.173 17.756 77.124 1.00 47.64 3673 C VAL B 826 40.130 16.5592 76.663 1.00 46.74 3673 C VAL B 826 41.363 21.236 77.651 1.00 46.61 3674 O VAL B 827 43.023 20.076 76.582 1.00 47.29 3676 CA MET B 827 44.025 21.031 77.139 1.00 48.46 3677 CB MET B 827 45.429 20.635 76.593 1.00 48.61 3679 SD MET B 827 43.641 22.449 76.548 1.00 55.19 3680 CE <td></td>										
3669 CA VAL B 826 40.825 19.160 76.439 1.00 46.21 3670 CB VAL B 826 41.173 17.756 77.124 1.00 46.13 3671 CGI VAL B 826 41.421 17.900 78.686 1.00 46.13 3673 C VAL B 826 41.762 20.239 76.958 1.00 46.74 3674 O VAL B 826 41.762 20.239 76.958 1.00 46.74 3675 N MET B 827 43.023 20.076 76.582 1.00 47.29 3677 CB MET B 827 46.036 19.261 77.139 1.00 48.46 3678 CG MET B 827 47.464 18.772 76.174 1.00 56.19 3680 CE MET B 827 43.641 22.449 76.548 1.00 50.13 3681 C <td></td>										
3670 CB VAL B 826 41.173 17.756 77.124 1.00 47.64 3671 CGI VAL B 826 41.421 17.900 78.686 1.00 48.86 3673 C VAL B 826 40.130 16.592 76.653 1.00 46.74 3674 O VAL B 826 41.363 21.236 77.651 1.00 46.74 3675 N MET B 827 43.023 20.076 76.582 1.00 47.23 3676 CA MET B 827 45.429 20.635 76.593 1.00 48.16 3678 CG MET B 827 45.429 20.635 76.593 1.00 48.13 3681 C MET B 827 43.641 22.447 76.548 1.00 53.80 3684 CA ALA B 828 43.175 22.647 75.280 1.00 50.45 3685 CB <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>1.00</td> <td>46.21</td>									1.00	46.21
3671 CG1 VAL B 826 41.421 17.900 78.686 1.00 46.13 3673 C VAL B 826 40.130 16.592 76.658 1.00 46.73 3674 O VAL B 826 41.363 21.236 77.651 1.00 46.61 3675 C MET B 827 43.023 20.076 76.582 1.00 47.29 3676 CA MET B 827 45.429 20.635 76.593 1.00 49.16 3679 SD MET B 827 46.036 19.261 77.139 1.00 56.19 3680 CE MET B 827 43.641 22.449 76.548 1.00 50.31 3681 C MET B 827 43.675 23.355 77.381 1.00 56.19 3683 N ALA B 828 42.467 24.49 76.548 1.00 50.45 3685 CB									1.00	47.64
3672 CG2 VAL B 826 41.762 20.239 76.958 1.00 46.74 3674 O VAL B 826 41.762 20.239 77.6551 1.00 46.74 3675 N MET B 827 43.023 20.076 76.582 1.00 47.29 3676 CA MET B 827 44.025 21.031 77.016 1.00 48.46 3678 CG MET B 827 45.429 20.635 76.593 1.00 49.16 3679 SD MET B 827 46.036 19.261 77.139 1.00 56.19 3680 CE MET B 827 43.641 22.449 76.548 1.00 50.31 3681 C MET B 828 43.175 22.647 75.280 1.00 50.45 3684 CA ALA B 828 41.656 <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>17.900</td> <td></td> <td>1.00</td> <td>46.13</td>							17.900		1.00	46.13
3673 C VAL B 26 41.363 21.236 76.958 1.00 46.61 3675 N MET B 827 43.023 20.076 76.582 1.00 46.61 3676 CA MET B 827 44.025 21.031 77.016 1.00 48.46 3678 CG MET B 827 46.036 19.261 77.139 1.00 48.13 3678 CG MET B 827 46.036 19.261 77.139 1.00 48.31 3680 CE MET B 827 43.641 22.449 76.548 1.00 50.31 3681 C MET B 827 43.675 23.355 77.381 1.00 50.45 3683 N ALA B 828 42.467 22.449 76.548 1.00 50.45 3685 CB ALA B 828 41.656		CG2	VAL	В	826		16.592	76.663	1.00	38.86
3675 N MET B 827 44.025 21.031 77.016 1.00 48.46 3676 CA MET B 827 44.025 21.031 77.016 1.00 48.46 3677 CB MET B 827 45.429 20.635 76.593 1.00 49.16 3678 CG MET B 827 46.036 19.261 77.139 1.00 56.19 3680 CE MET B 827 43.641 22.449 76.548 1.00 53.80 3681 C MET B 827 43.641 22.449 76.548 1.00 50.31 3682 O MET B 828 43.175 22.647 75.280 1.00 50.45 3683 N ALA B 828 42.467 24.087 73.404 1.00 49.04 3685 CB ALA B 828 41.656		С	VAL	В	826	41.762	20.239	76.958	1.00	46.74
3676 CA MET B 827 44.025 21.031 77.016 1.00 48.46 3677 CB MET B 827 45.429 20.635 76.593 1.00 49.16 3679 SD MET B 827 47.464 18.772 76.174 1.00 56.19 3680 CE MET B 827 43.641 22.449 76.548 1.00 50.380 3681 C MET B 827 43.675 23.355 77.381 1.00 51.02 3683 N ALA B 828 42.812 23.955 77.381 1.00 50.45 3684 CA ALA B 828 42.812 23.952 74.874 1.00 48.46 3685 CB ALA B 828 42.467 24.087 73.404 1.00 49.40 3687 O ALA B 828 41.656 24.425 75.727 1.00 45.93 3689 CA <td>3674</td> <td>0</td> <td>VAL</td> <td>В</td> <td>826</td> <td>41.363</td> <td>21.236</td> <td>77.651</td> <td>1.00</td> <td>46.61</td>	3674	0	VAL	В	826	41.363	21.236	77.651	1.00	46.61
3677 CB MET B 827 45.429 20.635 76.593 1.00 49.16 3678 CG MET B 827 46.036 19.261 77.139 1.00 48.31 3680 CE MET B 827 47.464 18.772 76.174 1.00 50.31 3681 C MET B 827 43.641 22.449 76.548 1.00 50.31 3682 O MET B 827 43.675 23.355 77.381 1.00 51.02 3683 N ALA B 828 42.467 24.087 73.404 1.00 49.40 3685 CB ALA B 828 41.656 24.425 75.727 1.00 47.69 3687 O ALA B 828 41.686 25.516 76.302 1.00 49.28 3689 CA ALA B 829 39.500	3675	N	MET	В	827	43.023	20.076	76.582	1.00	47.29
3678 CG MET B 827 47.464 18.772 76.174 1.00 56.19 3680 CE MET B 827 47.464 18.772 76.174 1.00 53.80 3681 C MET B 827 43.641 22.449 76.548 1.00 50.31 3682 O MET B 827 43.675 23.355 77.381 1.00 51.02 3683 N ALA B 828 43.175 22.647 75.280 1.00 50.45 3684 CA ALA B 828 42.467 24.087 73.404 1.00 49.40 3687 O ALA B 828 41.656 24.425 75.727 1.00 47.69 3689 CA ALA B 829 39.500 24.095 76.706 1.00 49.28 3691 C ALA B 829 39.974	3676	CA	MET	В	827	44.025	21.031	77.016	1.00	48.46
3679 SD MET B 47.464 18.772 76.174 1.00 56.19 3680 CE MET B 827 48.223 20.801 76.241 1.00 53.80 3681 C MET B 827 43.675 23.355 77.381 1.00 51.02 3683 N ALA B 828 43.175 22.647 75.280 1.00 50.45 3684 CA ALA B 828 42.812 23.992 74.874 1.00 48.64 3685 CB ALA B 828 41.656 24.425 75.727 1.00 47.69 3687 O ALA B 828 41.656 24.425 75.727 1.00 47.69 3688 N ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 39.428 25.519 <td>3677</td> <td>CB</td> <td>MET</td> <td>В</td> <td>827</td> <td>45.429</td> <td>20.635</td> <td>76.593</td> <td>1.00</td> <td>49.16</td>	3677	CB	MET	В	827	45.429	20.635	76.593	1.00	49.16
3680 CE MET B 827 48.223 20.801 76.241 1.00 53.80 3681 C MET B 827 43.641 22.449 76.548 1.00 50.31 3682 O MET B 827 43.675 23.355 77.381 1.00 50.45 3683 N ALA B 828 42.812 23.992 74.874 1.00 50.45 3685 CB ALA B 828 42.467 24.087 73.404 1.00 49.40 3687 O ALA B 828 41.656 24.425 75.727 1.00 47.69 3688 N ALA B 829 40.622 23.600 75.859 1.00 48.93 3689 CA ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 39.428 25.519 78.706 1.00 49.28 3691 C ALA B 829 39.428 25.519 78.706 1.00 50.99	3678	CG	MET	В	827	46.036	19.261	77.139	1.00	48.31
3681 C MET B 827 43.641 22.449 76.548 1.00 50.31 3682 O MET B 827 43.675 23.355 77.381 1.00 51.02 3683 N ALA B 828 42.812 23.992 74.874 1.00 48.64 3685 CB ALA B 828 42.467 24.087 73.404 1.00 49.40 3686 C ALA B 828 41.656 24.425 75.727 1.00 47.69 3687 O ALA B 828 41.656 24.425 75.727 1.00 47.69 3688 N ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 39.9500 24.095 76.877 1.00 48.53 3691 C ALA B 829 39.428 25.519 78.706 1.00 49.28 3693 N ILE B 830 40.902 23.804 78.674 1.00 54.22	3679	SD	MET	В	827	47.464	18.772	76.174	1.00	56.19
3682 O MET B 827 43.675 23.355 77.381 1.00 51.02 3683 N ALA B 828 43.175 22.647 75.280 1.00 50.45 3684 CA ALA B 828 42.812 23.992 74.874 1.00 49.40 3685 CB ALA B 828 42.467 24.087 73.404 1.00 49.40 3686 C ALA B 828 41.656 24.425 75.727 1.00 47.69 3687 O ALA B 829 40.622 23.600 75.859 1.00 48.34 3689 CA ALA B 829 39.500 24.095 76.6776 1.00 48.53 3691 C ALA B 829 39.974 24.564 78.107 1.00 50.69 3692 O ALA B 829 39.9428 25.519 78.706 1.00 52.39 3693 N ILE B 830 40.902 23.804 78.674 1.00 54.05 3695 CB ILE B 830 42.400 22.914 80.456 1.00 54	3680	CE	MET	В	827	48.223	20.801	76.241	1.00	53.80
3683 N ALA B 828 43.175 22.647 75.280 1.00 50.45 3684 CA ALA B 828 42.812 23.992 74.874 1.00 48.64 3685 CB ALA B 828 42.467 24.087 73.404 1.00 49.40 3687 O ALA B 828 41.656 24.425 75.727 1.00 47.69 3688 N ALA B 829 40.622 23.600 75.859 1.00 48.34 3689 CA ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 39.428 25.519 78.707 1.00 48.53 3691 C ALA B 829 39.428 25.519 78.707 1.00 51.92 3693 N ILE B 830 40.902 23.804 78.674 1.00 51.92 3695 CB	3681	C	MET	В	827	43.641	22.449	76.548	1.00	50.31
3684 CA ALA B 828 42.812 23.992 74.874 1.00 48.64 3685 CB ALA B 828 42.467 24.087 73.404 1.00 49.40 3686 C ALA B 828 41.656 24.425 75.727 1.00 47.69 3687 O ALA B 829 40.622 23.600 75.859 1.00 48.34 3688 CA ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 39.974 24.564 78.107 1.00 50.69 3691 C ALA B 829 39.974 24.564 78.107 1.00 50.69 3693 N ILE B 830 40.902 23.804 78.674 1.00 54.05 3695 CB ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB	3682	0	MET	В	827	43.675	23.355	77.381	1.00	51.02
3685 CB ALA B 828 42.467 24.087 73.404 1.00 49.40 3686 C ALA B 828 41.656 24.425 75.727 1.00 47.69 3687 O ALA B 828 41.688 25.516 76.302 1.00 45.93 3688 N ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 39.500 24.095 76.877 1.00 48.53 3691 C ALA B 829 39.428 25.519 78.706 1.00 50.69 3692 O ALA B 829 39.428 25.519 78.706 1.00 51.92 3693 N ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB ILE B 830 41.635	3683	N	ALA	В	828	43.175	22.647	75.280	1.00	50.45
3686 C ALA B 828 41.656 24.425 75.727 1.00 47.69 3687 O ALA B 828 41.688 25.516 76.302 1.00 45.93 3688 N ALA B 829 40.622 23.600 75.859 1.00 48.34 3689 CA ALA B 829 39.500 24.095 76.706 1.00 49.28 3691 C ALA B 829 39.974 24.564 78.107 1.00 50.69 3692 O ALA B 829 39.942 25.519 78.706 1.00 52.39 3693 N ILE B 830 40.902 23.804 78.674 1.00 51.92 3694 CA ILE B 830 42.400 22.914 80.456 1.00 54.22 3695 CB ILE B 830 41.635 21.788 81.139 1.00 55.56 3697 CD1	3684	CA	ALA	В	828	42.812	23.992	74.874	1.00	48.64
3687 O ALA B 828 41.688 25.516 76.302 1.00 45.93 3688 N ALA B 829 40.622 23.600 75.859 1.00 48.34 3689 CA ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 38.454 23.025 76.877 1.00 48.53 3691 C ALA B 829 39.428 25.519 78.706 1.00 52.39 3692 O ALA B 829 39.428 25.519 78.706 1.00 52.39 3693 N ILE B 830 40.902 23.804 78.674 1.00 51.92 3694 CA ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB ILE B 830 41.635 21.788 81.139 1.00 55.56 3697 CDI ILE	3685	CB	ALA	В	828	42.467	24.087	73.404	1.00	49.40
3688 N ALA B 829 40.622 23.600 75.859 1.00 48.34 3689 CA ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 38.454 23.025 76.877 1.00 48.53 3691 C ALA B 829 39.974 24.564 78.107 1.00 50.69 3692 O ALA B 829 39.428 25.519 78.706 1.00 52.39 3693 N ILE B 830 40.902 23.804 78.674 1.00 54.05 3695 CB ILE B 830 41.427 24.108 79.998 1.00 54.05 3696 CGI ILE B 830 41.635 21.788 81.139 1.00 55.66 3698 CG2 ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O ILE B <	3686	С	ALA	В	828	41.656	24.425	75.727	1.00	47.69
3689 CA ALA B 829 39.500 24.095 76.706 1.00 49.28 3690 CB ALA B 829 38.454 23.025 76.877 1.00 48.53 3691 C ALA B 829 39.974 24.564 78.107 1.00 50.69 3692 O ALA B 829 39.428 25.519 78.706 1.00 52.39 3693 N ILE B 830 40.902 23.804 78.674 1.00 51.92 3694 CA ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB ILE B 830 42.400 22.914 80.456 1.00 55.56 3697 CD1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O <td>3687</td> <td>0</td> <td>ALA</td> <td>В</td> <td>828</td> <td>41.688</td> <td>25.516</td> <td></td> <td></td> <td></td>	3687	0	ALA	В	828	41.688	25.516			
3690 CB ALA B 829 38.454 23.025 76.877 1.00 48.53 3691 C ALA B 829 39.974 24.564 78.107 1.00 50.69 3692 O ALA B 829 39.428 25.519 78.706 1.00 52.39 3693 N ILE B 830 40.902 23.804 78.674 1.00 51.92 3694 CA ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB ILE B 830 42.400 22.914 80.456 1.00 54.22 3696 CG1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 42.152 25.485 79.957 1.00 54.16 3699 C ILE B 830 41.872 26.417 80.751 1.00 54.16 3701 N ASN B 831 43.068 25.588 79.006 1.00 55.43 <td>3688</td> <td>N</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	3688	N								
3691 C ALA B 829 39.974 24.564 78.107 1.00 50.69 3692 O ALA B 829 39.428 25.519 78.706 1.00 52.39 3693 N ILE B 830 40.902 23.804 78.674 1.00 51.92 3694 CA ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB ILE B 830 42.400 22.914 80.456 1.00 54.22 3696 CG1 ILE B 830 41.635 21.788 81.139 1.00 55.56 3697 CD1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 43.521 23.378 81.390 1.00 52.02 3699 C ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O ILE B 830 41.872 26.417 80.751 1.00 54.16 3701 N ASN B 831 43.068 25.588 79.006 1.00 55.43 3702 CA ASN B 831 43.834 26.818 78.871 1.00 57.64 3703 CB ASN B 831 44.900 26.698 77.762 1.00 57.97 3704 CG ASN B 831 46.082 25.749 78.170 1.00 61.45 3705 OD1 ASN B 831 46.803 25.283 77.160 1.00 61.97 3707 C ASN B 831 46.803 25.283 77.160 1.00 61.97 3707 C ASN B 831 42.869 28.013 78.776 1.00 56.48 3708 O ASN B 831 43.088 29.055 79.374 1.00 57.73 3709 N ASP B 832 41.729 27.833 78.136 1.00 55.50 3710 CA ASP B 832 39.824 28.726 76.982 1.00 57.73 3711 CB ASP B 832 39.824 28.726 76.982 1.00 55.50 3712 CG ASP B 832 40.475 29.240 75.659 1.00 62.62 3713 OD1 ASP B 832 40.519 30.491 75.432 1.00 65.21 3714 OD2 ASP B 832 41.001 28.469 74.822 1.00 63.16	3689	CA	ALA	В	829	39.500				
3692 O ALA B 829 39.428 25.519 78.706 1.00 52.39 3693 N ILE B 830 40.902 23.804 78.674 1.00 51.92 3694 CA ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB ILE B 830 42.400 22.914 80.456 1.00 54.22 3696 CG1 ILE B 830 41.635 21.788 81.139 1.00 55.56 3697 CD1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 43.521 23.378 81.390 1.00 52.02 3699 C ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O ILE B 830 41.872 26.417 80.751 1.00 54.16 3701 N ASN B 831 43.068 25.588 79.006 1.00 55.43 3702 CA ASN B 831 43.834 26.818 78.871 1.00 57.64 3703 CB ASN B 831 44.900 26.698 77.762 1.00 57.97 3704 CG ASN B 831 46.082 25.749 78.170 1.00 61.45 3705 OD1 ASN B 831 46.082 25.749 78.170 1.00 61.45 3707 C ASN B 831 46.803 25.283 77.160 1.00 61.97 3707 C ASN B 831 43.088 29.055 79.374 1.00 57.73 3709 N ASP B 832 41.729 27.833 78.136 1.00 55.50 3710 CA ASP B 832 40.747 28.879 78.162 1.00 57.73 3710 CA ASP B 832 40.747 28.879 78.162 1.00 55.50 3711 CB ASP B 832 40.747 28.879 78.162 1.00 55.50 3712 CG ASP B 832 40.747 28.879 78.162 1.00 56.03 3712 CG ASP B 832 40.475 29.240 75.659 1.00 62.62 3713 OD1 ASP B 832 40.519 30.491 75.432 1.00 65.21 3714 OD2 ASP B 832 41.001 28.469 74.822 1.00 63.16 3715 C ASP B 832 39.956 28.914 79.478 1.00 53.83	3690									
3693 N ILE B 830 40.902 23.804 78.674 1.00 51.92 3694 CA ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB ILE B 830 42.400 22.914 80.456 1.00 54.22 3696 CG1 ILE B 830 41.635 21.788 81.139 1.00 55.56 3697 CD1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 43.521 23.378 81.390 1.00 52.02 3699 C ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O ILE B 830 41.872 26.417 80.751 1.00 54.16 3701 N ASN B 831 43.068 25.588 79.006 1.00 57.64 3703 CB ASN B 831 44.900 26.698 77.762 1.00 57.64 3704 CG ASN B 831 46.802 25.749 78.170 1.00 61.45		C								
3694 CA ILE B 830 41.427 24.108 79.998 1.00 54.05 3695 CB ILE B 830 42.400 22.914 80.456 1.00 54.22 3696 CG1 ILE B 830 41.635 21.788 81.139 1.00 55.56 3697 CD1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 43.521 23.378 81.390 1.00 52.02 3699 C ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O ILE B 830 41.872 26.417 80.751 1.00 54.16 3701 N ASN B 831 43.068 25.588 79.006 1.00 57.64 3703 CB ASN B 831 44.900 26.698 77.762 1.00 57.97 3704 CG ASN B 831 46.082 25.749 78.170 1.00 61.45 3705 OD1 ASN B 831 46.803 25.283 77.160 1.00 56.48 3708<		0								
3695 CB ILE B 830 42.400 22.914 80.456 1.00 54.22 3696 CG1 ILE B 830 41.635 21.788 81.139 1.00 55.56 3697 CD1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 43.521 23.378 81.390 1.00 52.02 3699 C ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O ILE B 830 41.872 26.417 80.751 1.00 54.16 3701 N ASN B 831 43.068 25.588 79.006 1.00 57.64 3703 CB ASN B 831 43.834 26.818 78.871 1.00 57.64 3703 CB ASN B 831 44.900 26.698 77.762 1.00 57.97 3704 CG ASN B 831 46.082 25.749 78.170 1.00 61.45 3705 OD1 ASN B 831 46.803 25.283 77.160 1										
3696 CG1 ILE B 830 41.635 21.788 81.139 1.00 55.56 3697 CD1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 43.521 23.378 81.390 1.00 52.02 3699 C ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O ILE B 830 41.872 26.417 80.751 1.00 54.16 3701 N ASN B 831 43.068 25.588 79.006 1.00 55.43 3702 CA ASN B 831 43.834 26.818 78.871 1.00 57.64 3703 CB ASN B 831 44.900 26.698 77.762 1.00 57.97 3704 CG ASN B 831 46.313 25.407 79.388 1.00 63.42 3705 OD1 ASN </td <td></td>										
3697 CD1 ILE B 830 40.775 22.243 82.301 1.00 56.62 3698 CG2 ILE B 830 43.521 23.378 81.390 1.00 52.02 3699 C ILE B 830 42.152 25.485 79.957 1.00 54.79 3700 O ILE B 830 41.872 26.417 80.751 1.00 54.16 3701 N ASN B 831 43.068 25.588 79.006 1.00 55.43 3702 CA ASN B 831 43.834 26.818 78.871 1.00 57.64 3703 CB ASN B 831 44.900 26.698 77.762 1.00 57.97 3704 CG ASN B 831 46.082 25.749 78.170 1.00 61.45 3705 OD1 ASN B 831 46.813 25.407 79.388 1.00 63.42 3706 ND2 ASN B 831 46.803 25.283 77.160 1.00 56.48 3708 O ASN B 831 43.088 29.055 79.374 1.00 57.73 3709 N ASP B 832 41.729 27.833 78.162 <td></td>										
3698										
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3702 CA ASN B 831 43.834 26.818 78.871 1.00 57.64 3703 CB ASN B 831 44.900 26.698 77.762 1.00 57.97 3704 CG ASN B 831 46.082 25.749 78.170 1.00 61.45 3705 OD1 ASN B 831 46.313 25.407 79.388 1.00 63.42 3706 ND2 ASN B 831 46.803 25.283 77.160 1.00 61.97 3707 C ASN B 831 42.869 28.013 78.776 1.00 56.48 3708 O ASN B 831 43.088 29.055 79.374 1.00 57.73 3709 N ASP B 832 41.729 27.833 78.136 1.00 55.50 3710 CA ASP B 832 40.747 28.879 78.162 1.00 54.22 3711 CB ASP B 832 40.475 29.240 75.659 1.00 62.62 3713 OD1 ASP B 832 40.519 30.491 75.432 1.00 65.21 3714 OD2 ASP B 832 41.001 28.469										
3703 CB ASN B 831										
3704 CG ASN B 831										
3705 OD1 ASN B 831 46.313 25.407 79.388 1.00 63.42 3706 ND2 ASN B 831 46.803 25.283 77.160 1.00 61.97 3707 C ASN B 831 42.869 28.013 78.776 1.00 56.48 3708 O ASN B 831 43.088 29.055 79.374 1.00 57.73 3709 N ASP B 832 41.729 27.833 78.136 1.00 55.50 3710 CA ASP B 832 40.747 28.879 78.162 1.00 54.22 3711 CB ASP B 832 39.824 28.726 76.982 1.00 56.03 3712 CG ASP B 832 40.475 29.240 75.659 1.00 62.62 3713 OD1 ASP B 832 40.519 30.491 75.432 1.00 65.21 3714 OD2 ASP </td <td></td>										
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3715 C ASP B 832 39.956 28.914 79.478 1.00 53.83										

FIGURE 3BV

A	В	С	D	E	F	G	Н	I	J
3717	N	GLY	В	833	40.258	28.009	80.431	1.00	52.62
3718	CA			833	39.487	28.103	81.674		52.59
3719	C			833	38.078	27.498	81.698		51.69
3720	0	GLY			37.252	27.863	82.546		53.45
3721	N			834	37.795	26.621	80.730	1.00	50.06
3722	CA			834	36.587	25.786	80.701		49.17
3723	СВ			834	36.577	24.912	79.451	1.00	46.71
3724	CG			834	35.397	23.934	79.392		49.59
3725	CD1	PHE	В	834	35.538	22.592	79.676		48.43
3726	CE1				34.451	21.720	79.632		49.88
3727	CZ	PHE	В	834	33.226	22.210	79.315	1.00	47.84
3728	CE2	PHE	В	834	33.106	23.517	78.977	1.00	49.60
3729	CD2	PHE	В	834	34.149	24.351	78.999	1.00	49.93
3730.	С	PHE	В	834	36.831	24.753	81.816	1.00	47.10
3731	0			834	37.960	24.368	82.076	1.00	46.20
3732	N			835	35.745	24.346	82.462	1.00	43.32
3733	CA	ARG	В	835	35.681	23.378	83.528	1.00	41.36
3734	CB	ARG	В	835	35.414	23.993	84.921	1.00	40.95
3735	CG	ARG	В	835	36.467	24.942	85.518	1.00	39.62
3736	CD	ARG	В	835	37.837	24.358	85.418	1.00	38.69
3737	NE	ARG	В	835	38.881	25.042	86.088	1.00	44.32
3738	CZ	ARG	В	835	39.934	25.489	85.438	1.00	50.44
3739	NH1	ARG			40.938	26.049	86.127	1.00	43.02
3740	NH2	ARG	В	835	39.981	25.329	84.088	1.00	44.62
3741	C	ARG	В	835	34.440	22.546	83.165	1.00	40.49
3742	0	ARG	В	835	33.483	23.057	82.604	1.00	41.54
3743	N	LEU	В	836	34.469	21.271	83.482	1.00	37.93
3744	CA	LEU	В	836	33.425	20.396	83.233	1.00	36.15
3745	CB	LEU	В	836	33.838	18.994	83.815	1.00	37.66
3746	CG	LEU	В	836	35.116	18.323	83.267	1.00	35.29
3747	CD1	LEU	В	836	35.499	17.005	83.929	1.00	33.23
3748	CD2	LEU	В	836	34.789	18.074	81.815	1.00	38.91
3749	C	LEU	В	836	32.232	20.956	83.981	1.00	36.97
3750	0	LEU	В	836	32.432	21.572	85.028	1.00	36.64
3751	N	PRO	В	837	30.999	20.719	83.525	1.00	34.28
3752	CA	PRO	В	837	29.824	21.275	84.187	1.00	34.92
3753	CB	PRO			28.789	21.273	83.072		34.34
3754	CG	PRO	В	837	29.449	20.600	81.871	1.00	39.22
3755	CD	PRO	В	837	30.650	19.919	82.344	1.00	35.63
3756	C	PRO	В	837	29.206	20.394	85.301		36.66
3757	0	PRO	В	837	29.462	19.205	85.411	1.00	34.31
3758	N	THR	В	838	28.308	20.910	86.081	1.00	37.44
3759	CA	THR	В	838	27.996	20.063	87.170		41.30
3760	CB	THR	В	838	27.125	20.677	88.173	1.00	42.22
3761	OG1	THR	В	838	26.152	19.670	88.570	1.00	45.09
3762	CG2	THR	В	838	26.224	21.773	87.502		44.87
3763	C	THR			27.248	18.908	86.572		43.03
3764	0	THR			26.534	19.021	85.578		44.86
3765	N	PRO			27.366	17.803	87.218		41.53
3766	CA	PRO			26.726	16.604	86.740		43.52
3767	CB	PRO			27.395	15.497	87.609		40.76
3768	CG	PRO	В	839	28.609	16.173	88.078	1.00	42.05

FIGURE 3BW

A	В	C	D	E	F	G	H	I	J
						•			
3769	CD	PRO	В	839	28.056	17.580	88.467	1.00	42.30
3770	C	PRO	В	839	25.278	16.789	87.071	1.00	44.34
3771	0	PRO	В	839	24.955	17.610	87.915	1.00	46.72
3772	N	ALA	В	840	24.416	16.004	86.466	1.00	46.17
3773	CA	ALA	В	840	22.989	16.149	86.701	1.00	46.30
3774	CB	ALA	В	840	22.229	15.193	85.735	1.00	46.61
3775	C	ALA	В	840	22.791	15.690	88.100	1.00	47.32
3776	0	ALA	В	840	23.359	14.659	88.452	1.00	48.03
3777	N	ASP	В	841	21.963	16.400	88.859	1.00	47.66
3778	CA	ASP	В	841	21.685	16.142	90.292		48.16
3779	CB			841	20.927	14.837	90.420	1.00	50.16
3780	CG	ASP	В	841	19.492	14.998	89.877	1.00	56.15
3781	OD1	ASP	В	841	18.696	13.990	89.914	1.00	57.77
3782	OD2	ASP			19.120	16.143	89.372	1.00	56.22
3783	C			841	22.863	16.166	91.204	1.00	47.22
3784	0	ASP	В	841	22.887	15.601	92.244	1.00	48.47
3785	Ň	CYS	В	842	23.875	16.886	90.866	1.00	45.42
3786	CA	CYS	В	842	24.882	16.890	91.830	1.00	42.29
3787	CB	CYS	В	842	26.202	17.117	91.137	1.00	42.38
3788	SG	CYS	В	842	27.632	17.081	92.149	1.00	39.32
3789	C	CYS	В	842	24.617	17.957	92.802	1.00	43.32
3790	0	CYS	В	842	24.280	19.092	92.452	1.00	45.03
3791	N	PRO	В	843	24.714	17.602	94.064	1.00	43.72
3792	CA	PRO	В	843	24.628	18.589	95.111	1.00	42.14
3793	CB	PRO	В	843	24.991	17.794	96.325	1.00	44.83
3794	CG	PRO	В	843	24.594	16.246	95.888	1.00	42.62
3795	CD	PRO	В	843	24.689	16.198	94.536	1.00	40.73
3796	C	PRO	В	843	25.658	19.593	94.858	1.00	42.60
3797	0	PRO	В	843	26.804	19.223	94.460	1.00	43.32
3798	N	SER	В	844	25.288	20.847	95.134	1.00	40.74
3799	CA	SER	В	844	26.138	22.019	94.922	1.00	41.10
3800	CB	SER	В	844	25.378	23.281	95.359	1.00	45.78
3801	OG	SER	В	844	24.007	22.921	95.667	1.00	47.77
3802	C	SER	В	844	27.363	22.044	95.753	1.00	39.64
3803	0	SER	В	844	28.384	22.625	95.348	1.00	40.26
3804	N	ALA	В	845	27.313	21.508	96.965		37.83
3805	CA	ALA			28.582	21.420	97.650	1.00	36.40
3806	CB	ALA	В	845	28.347	21.151	99.043	1.00	39.16
3807	C	ALA	В	845	29.485	20.414	97.041	1.00	36.50
3808	0	ALA	В	845	30.717	20.568	96.981	1.00	40.92
3809	N	ILE	В	846	28.983	19.393	96.448	1.00	37.49
3810	CA	ILE	В	846	29.931	18.505	95.824		38.19
3811	CB	ILE	В	846	29.123	17.228	95.389	1.00	38.40
3812	CG1	ILE	В	846	28.802	16.375	96.633	1.00	41.00
3813	CD1			846	30.056	16.440	97.794	1.00	34.53
3814	CG2			846	29.935	16.381	94.424		38.32
3815	C	ILE	В	846	30.488	19.261	94.613		39.49
3816	0			846	31.719	19.363	94.292	1.00	37.89
3817	N	TYR	В	847	29.540	19.759	93.833	1.00	42.21
3818	CA	TYR	В	847	30.006	20.529	92.653	1.00	42.74
3819	CB	TYR	В	847	28.846	21.081	91.802	1.00	43.60
3820	CG	TYR	В	847	29.434	21.686	90.506	1.00	46.75

FIGURE 3BX

A	В	С	D	E		F	G	Н	I	J
3821	CD1	TYR	R	847		29.238	23.035	90.142	1.00	40.15
3822	CE1	TYR		847		29.804	23.528	88.926	1.00	48.32
3823	CZ	TYR		847		30.561	22.684	88.120		44.77
3824	OH	TYR		847		31.151	23.079	86.988		40.40
3825	CE2	TYR		847		30.776	21.358	88.509	1.00	
3826	CD2	TYR		847		30.234	20.893	89.685		47.08
3827	C,	TYR		847		30.858	21.662	93.143		40.26
3828	0	TYR		847		31.963	21.877	92.659		40.34
3829	N	GLN		848		30.451	22.340	94.207		41.30
3830	CA	GLN		848		31.418	23.410	94.664	1.00	
3831	CB	GLN	В	848		30.823	24.320	95.701	1.00	45.07
3832	CG	GLN	В	848		31.676	25.537	96.106	1.00	51.95
3833	CD	GLN		848		31.283	26.899	95.372	1.00	63.54
3834	OE1	GLN		848		30.417	26.923	94.412	1.00	64.88
3835	NE2	GLN		848		31.976	28.042	95.806	1.00	60.42
3836	C	GLN	В	848		32.850	22.934	94.967	1.00	41.04
3837	0	GLN	В	848		33.897	23.527	94.527	1.00	41.33
3838	N	LEU	В	849		32.915	21.786	95.608	1.00	38.01
3839	CA	LEU	В	849		34.208	21.204	95.905	1.00	35.47
3840	CB	LEU	В	849		33.889	20.040	96.868	1.00	36.49
3841	CG	LEU	В	849		35.120	19.349	97.222	1.00	36.62
3842	CD1	LEU	В	849		36.078	20.393	97.866	1.00	32.52
3843	CD2	LEU	В	849		34.708	18.241	98.241	1.00	43.70
3844	C	LEU	В	849		34.946	20.716	94.708	1.00	35.06
3845	0	LEU	В	849		36.200	20.891	94.564	1.00	34.28
3846	N	MET	В	850		34.223	20.003	93.821	1.00	35.02
3847	CA	MET	В	850		34.861	19.681	92.512	1.00	36.09
3848	CB	MET	В	850		33.703	19.134	91.632	1.00	37.35
3849	CG	MET	В	850		33.905	18.476	90.380	1.00	32.97
3850	SD	MET	В	850		32.372	17.871	89.923	1.00	36.02
3851	CE	MET	В	850		31.755	17.245	91.136	1.00	32.09
3852	C	MET	В	850		35.487	21.062	92.000	1.00	36.72
3853	0	MET	В	850		36.645	21.219	91.693	1.00	38.32
3854	N	MET	В	851		34.747	22.126	91.975	1.00	37.60
3855	CA	MET	В	851		35.408	23.296	91.429	1.00	38.96
3856	CB	MET	В	851		34.424	24.425	91.381	1.00	38.34
3857	CG	MET	В	851		33.322	24.168	90.395	1.00	38.17
3858	SD	MET	В	851		33.760	24.269	88.645		45.90
3859	CE			851		34.669	25.672	88.676		46.07
3860	C	MET	В	851		36.688	23.732	92.181	1.00	41.53
3861	0	MET	В	851		37.765	24.106	91.542		43.20
3862	N			852		36,617	23.715	93.495		38.35
3863	CA	GLN	В	852		37.772	24.172	94.206		39.33
3864	CB			852		37.474	24.264	95.703		42.34
3865	CG			852		36.356	25.195	96.036		45.28
3866	CD			852	•	35.754	24.863	97.391		62.60
3867	OE1					34.797	25.545	97.871		68.59
3868	NE2	GLN				36.292	23.806	98.030		69.44
3869	C			852		38.834	23.236	93.879		40.26
3870	0			852		39.939	23.631	93.706		41.90
3871	N			853		38.590	21.960	93.648		40.71
3872	CA	CYS	В	853		39.835	21.254	93.263	1.00	39.23

FIGURE 3BY

A	В	С	D	E	F	G	Н	I	J
3873	СВ	CYS	В	853	39.782	19.711	93.273	1.00	39.20
3874	SG			853	38.918	18.954	94.690	1.00	40.47
3875	С			853	40.318	21.686	91.913	1.00	40.72
3876	0			853	41.421	21.347	91.564	1.00	38.66
3877	N			854	39.519	22.366	91.092	1.00	41.68
3878	CA	TRP	В	854	40.111	22.647	89.772	1.00	44.18
3879	CB	TRP	В	854	39.031	22.457	88.667	1.00	44.45
3880	CG	TRP	В	854	38.618	21.114	88.501	1.00	41.82
3881	CD1	TRP	В	854	39.368	19.980	88.704	1.00	41.87
3882	NE1			854	38.602	18.866	88.449		35.93
3883	CE2			854	37.352	19.263	88.140		32.47
3884	CD2	TRP	В	854	37.333	20.687	88.167		38.06
3885	CE3			854	36.138	21.359	87.897		32.76
3886	CZ3			854	35.127	20.665	87.536		29.91
3887	CH2			854	35.159	19.211	87.528		36.45
3888	CZ2			854	36.282	18.524	87.789		32.15
3889	C			854	40.722	24.083	89.583		45.26
3890	0			854	41.080	24.493	88.441		43.51
3891	N	GLN		855	40.727	24.844	90.675		45.68
3892	CA	GLN		855	41.226	26.182	90.651		46.55
3893	CB			855	41.379	26.724	92.049		48.28 50.56
3894	CG CD	GLN		855 855	40.053 40.145	26.999	92.625 93.423		60.72
3895 3896	OE1			855	40.143	28.208 28.135	94.670		58.07
3897	NE2			855	40.024	29.384	92.729		61.21
3898	C	GLN		855	42.519	26.130	90.037		45.75
3899	0			855	43.278	25.307	90.342		42.80
3900	N			856	42.710	27.051	89.106		47.78
3901	CA			856	43.924	27.243	88.368		47.38
3902	CB			856	43.729	28.485	87.470		49.87
3903	CG	GLN	В	856	44.834	28.698	86.488	1.00	49.20
3904	CD	GLN	В	856	44.839	27.597	85.453	1.00	59.89
3905	OE1	GLN	В	856	43.788	26.947	85.185	1.00	61.37
3906	NE2	GLN	В	856	46.017	27.356	84.866	1.00	60.84
3907	C	GLN	В	856	45.065	27.456	89.331	1.00	46.71
3908	0	GLN	В	856	46.106	26.883	89.154		44.54
3909	N			857	44.892	28.308	90.331		48.11
3910		GLU				28.408	91.341		51.65
3911	CB			857	45.768	29.578	92.387		52.14
3912	CG			857	46.166	30.915	91.710		62.33
3913	CD			857	45.832	32.252	92.398		71.26
3914		GLU			45.616	32.369	93.641		76.69
3915		GLU			45.828	33.239	91.631		75.04
3916	C			857	46.160	27.138	92.117		49.78
3917	O N			857 858	45.368	26.874 26.345	93.003 91.823		50.77 48.84
3918 3919	N CA	ARG ARG			47.167 47.332	25.179	92.679		48.89
3919	CB	ARG			48.631	24.421	92.402		48.75
3921	CG			858	49.933	24.995	92.988		46.77
3922	CD			858	51.166	24.444	92.169		55.09
3923	NE			858	52.374		92.946		66.77
3924	CZ			858	53.580	24.706	92.706		70.86
			_						

FIGURE 3BZ

A	В	С	D	E	F	G	Н	I	J
3925	NH1	ARG	В	858	53.804	25.519	91.672	1.00	68.19
3926	NH2	ARG		858	54.588	24.373	93.510	1.00	75.23
3927	C	ARG		858	47.192	25.455	94.211	1.00	49.58
3928	0	ARG		858	46.606	24.640	94.922	1.00	47.02
3929	N	ALA		859	47.743	26.584	94.704	1.00	49.56
3930	CA	ALA	В	859	47.766	26.775	96.131	1.00	49.75
3931	CB	ALA	В	859	48.584	27.954	96.533	1.00	51.56
3932	C	ALA	В	859	46.364	26.871	96.691	1.00	49.92
3933	0	ALA	В	859	46.123	26.666	97.946	1.00	47.88
3934	N	ALA	В	860	45.410	27.081	95.789	1.00	47.89
3935	CA	ALA	В	860	44.084	27.368	96.360	1.00	46.93
3936	CB	ALA	В	860	43.377	28.492	95.576	1.00	48.07
3937	C	ALA	В	860	43.240	26.131	96.356	1.00	45.49
3938	0	ALA		860	42.064	26.182	96.738	1.00	43.79
3939	N	ARG	В	861	43.808	25.041	95.824	1.00	
3940	CA	ARG		861	43.069	23.742	95.850		45.03
3941	CB	ARG		861	43.616	22.678	94.889	1.00	45.11
3942	CG			861	43.572	23.172	93.351	1.00	46.90
3943	CD	ARG		861	44.345	22.261	92.433	1.00	44.77
3944	NE	ARG		861	44.743	22.970	91.264	1.00	38.07
3945	CZ	ARG		861	45.809	22.714	90.575	1.00	41.87
3946	NH1	ARG		861	46.592	21.700	90.905	1.00	38.56
3947	NH2	ARG		861	46.150	23.523	89.537	1.00	43.27
3948	C	ARG		861	43.130	23.309	97.271		45.07
3949	0	ARG		861	44.103	23.626	98.032		44.45
3950 3951	N CA	PRO PRO		862 862	42.026 41.895	22.694 22.193	97.660 98.984	1.00 1:00	43.87
3951	CB	PRO		862	40.554	21.463	98.980	1.00	44.25
3953	CG	PRO		862	39.896	21.403	97.717	1.00	41.03
3954	CD	PRO		862	40.829	22.473	96.845	1.00	44.03
3955	C	PRO		862	42.931	21.188	99.086	1.00	43.12
3956	Ō	PRO		862	43.244	20.570	98.142		42.37
3957	N			863	43.431	21.006	100.274		43.78
3958	CA	LYS			44.308	19.872	100.517	1.00	44.01
3959	CB	LYS	В	863	45.168	20.223	101.764	1.00	44.71
3960	CG	LYS	В	863	46.523	20.788	101.339	1.00	51.54
3961	CD	LYS	В	863	46.460	22.176	100.652	1.00	56.44
3962	CE	LYS	В	863	47.864	22.699	100.246	1.00	61.29
3963	NZ	LYS	В	863	49.033	21.667	100.373	1.00	67.02
3964	C	LYS	В	863	43.545		100.706	1.00	39.71
3965	0	LYS	В	863	42.327		101.170	1.00	38.33
3966	N	PHE	В	864	44.230		100.460		36.76
3967	CA	PHE	В	864	43.420	16.152	100.759		38.90
3968	CB			864	44.140		100.429		37.94
3969	CG			864	44.178	14.527	98.922		33.91
3970		PHE			45.375	14.533			29.69
3971		PHE			45.459	14.319	96.835		34.24
3972	CZ	PHE			44.247	14.052	96.097		34.64
3973		PHE			43.040	14.039	96.796		34.40
3974		PHE			43.011	14.281	98.235		33.00
3975	C			864	42.796		102.134		39.31
3976	0	PHE	В	864	41.644	15.610	102.340	1.00	42.22

FIGURE 3CA

A	В	C	D	E	F	G	H	I	J
			_						
3977	N			865	43.535	16.632	103.081		38.65
3978	CA			865	43.021		104.387		41.81
3979	CB			865	44.179	16.905	105.512		42.20
3980	C			865	41.864		104.488		41.60
3981	0	ALA		865	40.936		105.218		41.67
3982	N			866	41.882		103.846		42.39
3983	CA	ASP		866	40.590	19.411	104.022		44.31
3984	CB			866	40.540		103.439		44.90
3985	CG			866	41.770		103.675		50.05
3986	OD1	ASP			42.078		104.884		55.78
3987	OD2	ASP			42.487		102.707		49.26
3988	C			866	39.398		103.357		43.11
3989	0			866	38.289		103.908		40.88
3990	N G7	ILE		867	39.687	17.950	102.214		41.48
3991	CA			867	38.644	17.260	101.454		39.52
3992	CB			867	39.235	16.640	100.175		39.26
3993 3994	CG1			867	39.557	17.782	99.199		37.38
3995	CD1 CG2			867	40.457	17.388	97.911	1.00	34.65
3996	CGZ			867 867	38.265	15.618	99.527	1.00	30.26
3997	0			867	38.010 36.787	16.203 16.055	102.272	.1.00	39.36 37.24
3998	N			868	38.841	15.458	102.304		40.82
3999	CA			868	38.200		102.900		40.82
4000	CB			868	39.269		103.509		43.83
4001	CG1			868	38.560		105.520		38.82
4001	CG2	VAL			40.125		103.520		39.45
4002	C			868	37.345		104.808		40.69
4004	0			868	36.193		105.003	1.00	
4005	N			869	37.826		105.485		41.17
4006	CA			869	36.879	16.666	106.516		44.54
4007	CB			869	37.479	17.651	107.541		46.64
4008	OG			869	38.536	18.378	106.941		50.61
4009	C			869	35.713		105.912		44.10
4010	0			869	34.559		106.449		45.09
4011	N			870	35.941	17.977	104.771		43.54
4012	CA			870	34.744	18.495	104.139		42.08
4013	СВ	ILE	В	870	34.755	19.950	103.300		43.22
4014	CG1			870	33.586	19.999	102.312	1.00	41.61
4015	CD1	ILE	В	870	33.949	19.365	101.176		41.32
4016	CG2	ILE	В	870	36.033	20.464	102.635		40.07
4017	С	ILE			33.864	17.382	103.682	1.00	41.89
4018	0	ILE	В	870	32.658		103.793		41.51
4019	N	LEU	В	871	34.404	16.281	103.192		42.27
4020	CA	LEU	В	871	33.374	15.249	102.861	1.00	42.82
4021	CB	LEU	В	871	33.923	14.113	101.973		40.18
4022	CG	LEU			34.172	14.656	100.580	1.00	
4023	CD1	LEU		871	34.974	13.645	99.846		42.97
4024	CD2	LEU		871	32.952	15.032	99.820	1.00	30.76
4025	С	LEU	В	871	32.699		104.115		41.38
4026	0	LEU	В	871	31.528	14.182	104.128		43.91
4027	N	ASP			33.394		105.207		41.15
4028	CA	ASP	В	872	32.653	14.052	106.384	1.00	41.49

FIGURE 3CB

A	В	С	D	E	F	G	Н	I	J
4029	СВ	ASP	R	872	33.673	13.713	107.437	1.00	39.80
4030	CG			872	34.462	12.401	107.107		45.40
4031		ASP		872	33.894	11.494			51.78
4032		ASP		872	35.617	12.127		1.00	
4033	C	ASP		872	31.402	14.875	106.910	1.00	
4034	Ö	ASP		872	30.268	14.269	107.347	1.00	42.17
4035	N	LYS		873	31.557	16.226	106.813	1.00	
4036	CA	LYS		873	30.499	17.147		1.00	
4037	СВ	LYS		873	30.925	18.620	107.369	1.00	46.52
4038	CG	LYS		873	32.038	18.846		1.00	52.07
4039	CD			873	32.946		107.986	1.00	60.03
4040	CE			873	33.740	20.457			66.29
4041	NZ	LYS	В	873	34.221	19.164	109.838	1.00	72.68
4042	C			873	29.324	17.049	106.377	1.00	47.08
4043	0	LYS	В	873	28.196	17.131	106.833	1.00	48.85
4044	N	LEU	В	874	29.503	16.815	105.094	1.00	46.56
4045	CA	LEU	В	874	28.235	16.640	104.425	1.00	45.19
4046	CB	LEU	В	874	28.375	16.817	102.875	1.00	46.34
4047	CG	LEU	В	874	29.232	18.022	102.434	1.00	48.30
4048	CD1	LEU	В	874	29.940	17.832	101.164	1.00	45.32
4049	CD2	LEU	В	874	28.475	19.386	102.439	1.00	51.85
4050	C	LEU	В	874	27.677	15.295	104.767	1.00	46.11
4051	0	LEU	В	874	26.433	15.095	104.797	1.00	42.90
4052	N	ILE	В	875	28.568	14.289	104.846	1.00	48.45
4053	CA	ILE	В	875	28.076	12.933	105.024	1.00	49.62
4054	CB	ILE	В	875	29.276	11.927	105.013	1.00	50.00
4055	CG1	ILE	В	875	29.557	11.427	103.630	1.00	49.38
4056	CD1	ILE	В	875	30.973	10.853	103.455	1.00	
4057	CG2	ILE	В	875	29.010	10.708	105.957		48.28
4058	C			875	27.452		106.397	1.00	
4059	0	ILE			26.435	12.478	106.683	1.00	52.10
4060	N			876	28.026	13.876		1.00	55.97
4061	CA	ARG		876	27.371		108.590	1.00	
4062	CB	ARG		876	28.395	14.347			60.00
4063	CG	ARG		876	28.796		110.592	1.00	61.19
4064	CD	ARG		876	29.309		110.037	1.00	67.05
4065	NE			876	30.770		110.044	1.00	76.99
4066	CZ				31.568		111.116		
4067		ARG			32.887		110.939		81.01
4068		ARG			31.067		112.335		79.88
4069	C	ARG			26.149		108.667		61.31
4070	0			876	25.336		109.576		63.40
4071	N			877	25.990		107.728		61.95 60.39
4072	CA CB			877	24.782		107.724		61.56
4073 4074	CB	ALA		877	25.142		108.099 106.334		60.30
4074	0	ALA			24.104 24.050		105.548		59.22
4075	N			878	23.522		105.546		60.43
4078	CA			878	23.006		104.833		60.78
4077	CB			878	22.159		104.833		60.78
4078	CG			878.	22.139		105.162		59.55
4079	CD			878	23.223		100.336		61.36
±000	CD	FKU	ם	0/0	43.443	14.400	107.133	1.00	01.50

FIGURE 3CC

A	В	С	D	E	F	G .	Н	I	J
4081	C	PRO	В	878	22.093	16.025	104.243	1.00	60.68
4082	Ö	PRO			21.843	15.907	103.015	1.00	60.12
4083	N	ASP		879	21.492	16.871	105.081	1.00	59.38
4084	CA	ASP	В	879	20.644	17.925	104.532	1.00	59.16
4085	CB	ASP	В	879	19.959	18.741	105.618	1.00	59.04
4086	CG	ASP		879	18.427		105.571	1.00	66.19
4087	OD1		В	879	17.726	19.586	105.290	1.00	72.48
4088	OD2	ASP	В	879	17.829	17.463	105.707	1.00	71.81
4089	C	ASP	В	879	21.462	18.826	103.603	1.00	57.43
4090	0	ASP	В	879	20.981	19.301	102.590	1.00	57.64
4091	N	SER	В	880	22.716	19.032	103.975	1.00	56.33
4092	CA	SER	В	880	23.644	19.836	103.267	1.00	54.79
4093	CB	SER	В	880	24.929	19.797	104.005	1.00	55.24
4094	OG	SER	В	880	25.622	18.605	103.690	1.00	55.50
4095	C	SER	В	880	23.879	19.301	101.868	1.00	54.99
4096	0	SER	В	880	24.507	19.979	101.077	1.00	53.72
4097	N	LEU	В	881	23.348	18.113	101.566	1.00	55.55
4098	CA	LEU	В	881	23.478	17.516	100.243	1.00	56.64
4099	CB	LEU	В	881	23.957	16.066	100.370	1.00	55.16
4100	CG	LEU	В	881	25.385	16.073	100.877	1.00	47.41
4101	CD1	LEU	В	881	25.879	14.711	101.097	1.00	44.25
4102	CD2	LEU		881	26.234	16.645	99.827	1.00	38.61
4103	C	LEU		881	22.260	17.570	99.338	1.00	60.26
4104	0	LEU		881	22.311	17.141	98.189	1.00	61.01
4105	N	ALA	В	882	21.141	18.068	99.839	1.00	64.54
4106	CA	ALA			19.923	18.077	99.007	1.00	66.81
4107	CB	ALA		882	18.619	18.004	99.875	1.00	66.76
4108	C	ALA		882	19.875	19.245	98.028	1.00	68.16
4109	0	ALA		882	19.531	19.064	96.866	1.00	69.24
4110	N	ALA		883	20.126	20.446	98.515	1.00	68.60
4111	CA	ALA		883	20.325	21.591	97.630	1.00	69.28
4112	CB	ALA			20.372	22.901	98.461	1.00	69.49
4113	C	ALA			21.685	21.361	96.886	1.00	69.14
4114	0	ALA			21.818	21.511	95.652	1.00	68.44
4146		ATP		1001	46.712	-3.440	86.953	1.00	89.49
4147	PA	ATP		1001	45.850	-2.328	86.523	1.00	84.33
4148		ATP			45.971	-1.113	87.512	1.00	78.95
4149		ATP			46.316	-2.240	84.993 84.575		89.69 98.93
4150	PB	ATP ATP			47.730				99.05
4151 4152		ATP			48.070 48.948				95.56
		ATP			47.340				
4153 4154	PG	ATP			45.810				101.51
4155		ATP			45.916				97.15
4156		ATP			45.159				95.81
4157		ATP			44.985				99.53
4157		ATP			44.345				81.43
4159		ATP			44.056		85.310		76.05
4160		ATP			42.586				72.65
4161		ATP			42.294				66.71
4162		ATP			41.362				60.60
4163		ATP			40.769				62.85
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FIGURE 3CD

A	В	C	D	E	F	G	Н	I	J
4164	02*	ATP	В1	001	40.111	-3.69	4 85.576	1.00	60.83
4165	C3*	ATP	В1	001	42.005	-3.00	4 86.424	1.00	67.86
4166	03*	ATP	В1	001	41.724	-1.88	4 85.612	1.00	68.16
4167	N9	ATP	В1	001	42.167	-5.20	2 88.434	1.00	53.63
4168	C8	ATP	В1	001	43.500	-4.81	3 88.655	1.00	53.17
4169	N7	ATP	В1	001	43.833	-5.10	8 89.970	1.00	50.95
4170	C5	ATP	В1	001	42.701	-5.61	2 90.619	1.00	46.80
4171	C6	ATP	В1	001	42.436	-6.00	5 91.949	1.00	44.40
4172	N6	ATP	В1	001	43.185	-5.60	0 93.067	1.00	37.97
4173	C4	ATP	В1	001	41.684	-5.68	7 89.652	1.00	48.42
4174	N3	ATP	В1	001	40.432	-6.10	8 89.965	1.00	44.97
4175	C2	ATP	В1	001	40.181	-6.52	9 91.253	1.00	46.46
4176	N1	ATP	В1	001	41.180	-6.52	2 92.179	1.00	41.31